I U C L I D

Data Set

Existing Chemical	:	ID: 1918-00-9
Memo	:	TRA
CAS No.	:	1918-00-9
Generic name	:	2-methoxy-3,6-dichlorobenzoic acid
Synonym	:	3,6-dichloro-o-anisic acid
Product name	:	dicamba

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	87 - 108 °C
Sublimation	:	
Method	:	OECD Guide-line 102 "Melting Point/Melting Range"
Year	:	1981
GLP	:	yes
Test substance	:	

Method : Test was performed according to OECD 102, capillary method - metal block apparatus.

Two capillary tubes containing finely ground test substance were tested simultaneously (determination 1 and 2). Melting point of acetanilide was measured to determine the accuracy of the apparatus before the actual test.

Result :

	determination 1	determination 2
beginning of melting (deg C)	87	87
final stage of	108	108

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (dicamba, technical), purity 85.9% (by HPLC)
Conclusion	:	melting range is 87-108 deg C
Reliability	:	(1) valid without restriction No results for the reference substance are given. However, accuracy was estimated to be 0.5 deg C which is by far exceeded by the length of the temperature range.
Flag	:	Critical study for SIDS endpoint

25.12.2001 (12)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	.0000167 hPa at 25 °C
Decomposition	:	ambiguous
Method	:	other (measured): US EPA Pesticide Assessment Guidelines (40 CFR 158), Subdivision D, No 63-9. Essentially OECD 104, gas saturation method.
Year	:	
GLP	:	yes
Test substance	:	other TS

Method : VP was determined at 8 different temperatures between 95 and 111 deg C using a Dupont 916 Thermal Evolution Analyzer. Using this apparatus, test substance saturation in a carrier gas is achieved at a certain temperature. The gas chamber effluent is swept to an on-line coupled Flame Ionization Detector, the response of which is proportional to the number of moles of TS reaching the detector per unit of time. TS (0.1061 g) was loaded on sea sand (0.9373 g). Nitrogen was used as carrier gas; VP was determined at 3 flow rates (0.680, 1.858 and 3.893 mL/min) for each

temperature. Validity of the method was determined using dimethylphthalate as a reference substance.
VP at 25 deg C was determined by extrapolation of a log VP vs. 1000/T line.

Remark : The vapor pressure is supported by the EPIWIN v3.05 calculated value of 0.0000075 hPa.

Result : Temperature (deg C) / Average empirical VP (mm Hg)

Temperature (deg C)	Average empirical VP (mm Hg)
95	0.1080
97	0.1281
99	0.1500
100	0.1796
104	0.2558
106	0.3209
110	0.4512
111	0.5471

Log VP = -6145.6/T (K) + 15.7189 (mm Hg)
with T(K) = t(deg C) + 273
(correlation coefficient = -0.9980)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : I, CAS 1918-00-9 (dicamba), purity 99.18% (HPLC)
Conclusion VP at 25 deg C = 1.25E-5 mm Hg (1.67E-5 hPa)
Reliability : (2) valid with restrictions
Extrapolation from 95 deg C as lowest T to 25 deg C may cause a relative error since, at 95 deg C TS may be partially fluid, whereas at 25 deg C it is a solid. Extrapolation may therefore be problemetic. It is, however, the best possible option under these circumstances.
Flag : Critical study for SIDS endpoint
25.12.2001 (12) (14)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : = 2.21 at °C
pH value :

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1918-00-9 (dicamba)
Reliability : (2) valid with restrictions
Score of 2 given to handbook or published values for physical constants. The measured value in the other listed study is for the partially ionized form of the TS.
Flag : Critical study for SIDS endpoint
25.12.2001 (4)

Partition coefficient :
Log pow : .545 at 25 °C
pH value :
Method : other (measured): EPA Pesticide Assessment Guidelines, Subdivision D, Product Chemistry, Section 63-11. Essentially OECD 107
Year : 1982
GLP : yes
Test substance : other TS

Method : Because test substance dissociates in aqueous and octanol phase, Kow of non-dissociated TS was calculated on basis of measured test substance concentrations and pH of the two

phases and on pKa of the test substance (1.94).

0.497 mg and 5.054 mg test substance (specific activities 1.28E6 dpm/mg and 1.26E5 dpm/mg, respectively) were each dissolved in 5 mL buffer-presaturated n-octanol after which 5 mL n-octanol-presaturated buffer was added. The mixtures were shaken in a water bath at 25 deg C for 1 hour, centrifuged (2000 rpm, 20 min) and duplicate 1.0 mL aliquots were taken from both phases and analyzed by LSC. The pH of each phase was measured.
Three buffer solutions of pH 5.0, 7.0 and 9.0 were used. For each pH and each TS concentration triplicate test mixtures were prepared.
The fraction of undissociated dicamba in each phase was calculated on basis of measured ion concentration, pKa and pH.

Result : Buffer pH | Initial TS concentration in n-octanol (mM) | Kow (mean of 3 replicates)

Buffer pH	Initial TS concentration in n-octanol (mM)	Kow (mean of 3 replicates)
5.0	4.58	6.86 +/- 0.60
7.0	4.58	0.54 +/- 0.01
9.0	4.58	8.95 +/- 0.06
5.0	0.499	3.98 +/- 0.11
7.0	0.499	0.16 +/- 0.00
9.0	0.499	0.58 +/- 0.00

Average Kow: 3.51 +/- 3.73

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (dicamba), analytical reference standard
I, CAS 1918-00-9 (14C-dicamba), radiochemical purity 98%

Conclusion : Kow of test substance strongly depends on pH and on test substance concentration.
Kow ranged between 0.2 and 9.0.

Reliability : (2) valid with restrictions
1. Measurement was performed on ionized form of TS, which results in deviations from the partition law. Measurement should have been performed on non-ionized TS and therefore at low pH. OECD 107 suggests pH at least one unit below pKa. However, as pKa = 1.94 pH should have been < 1 which is very low. Therefore, this has to be considered best possible method.
2. Only one n-octanol: water ratio was tested for each pH and concentration.

25.12.2001 (15)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : 8.24 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : soluble (1000-10000 mg/L)
Stable :
Deg. product :

Method	:	other: essentially OECD 105 (flask method)
Year	:	1993
GLP	:	yes
Test substance	:	other TS
Method	:	25 mL water of Milli-Q reagent grade were added to 0.50 g test substance. The mixture was shaken for about one hour and was then placed in a water bath (25 deg C) for at least 48 hrs. With intervals of at least 24 h the mixture was centrifuged and returned to a waterbath (25 deg C) for temperature equilibration (at least 1 h). The test solutions were analyzed in duplicate using HPLC against dicamba calibration standards (dicamba in methanol, 1.028-10.285 mg/mL). Measurements were repeated until SD of the two last measurements was within the method reproducibility.
Remark	:	This value is supported by a vlaue of 6500 mg/L at 25 C given by: Tomlin, C.D.S. (ed.). The Pesticide Manual - World Compendium. 10th ed. Surrey, UK: The British Crop Protection Council, 1994. 298 (as cited in Hazardous Substance Data Base)
Result	:	Solubility in water at 25 deg C: 0.824 g per 100 mL solution
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (dicamba, technical), purity 85.9%
Conclusion	:	Solubility of test substance in water is 8.24 g/L.
Reliability	:	(2) valid with restrictions 1. Only the end result is reported, no individual results of measurements are given. Results can therefore not be checked. 2. Method is intended for essentially pure chemicals. Dicamba technical cannot be regarded as such. 3. It should be noted that whereas technical dicamba was tested, a reference standard of 99.18% purity was used for calibration. Impurities have therefore been disregarded.
Flag	:	Critical study for SIDS endpoint

25.12.2001 (13)

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Xenon lamp
Light spectrum	:	> 290 nm
Relative intensity	:	1.32 based on intensity of sunlight
Conc. of substance	:	100.19 mg/l at 25 °C
DIRECT PHOTOLYSIS		
Halflife t1/2	:	50.3 day(s)
Degradation	:	31.3 % after 30 day(s)
Quantum yield	:	
Deg. product	:	yes
Method	:	EPA Guide-line subdivision N 161-2 "Photodegradation studies in water"
Year	:	1982
GLP	:	yes
Test substance	:	other TS

Method :

A 1000 mL test solution consisting of 100.19 mg dicamba with a specific activity of 412.2 dpm/ug (total 688 kBq) in aqueous buffer solution pH 7 containing 1% acetonitrile was prepared. The test solution was incubated at 25 +/- 1 deg C under contineous stirring for 30 days. Average incident radiation on the reactor surface was 7.704E2 W/m2 (measured before and after the study).
The reaction solution was aerated and connected to a silica gel trap, an ethylene glycol trap (organic volatiles) and a 10% NaOH trap (supposed to collect CO2) in series. Before initiation of photolysis, a 50 mL sample was taken as dark control sample. 20 mL samples were taken before initiation of photolysis and on day 1, 3, 8, 15, 22 and 30.

The samples were analyzed as follows:
- duplicate 1 mL samples were analyzed by LSC
- 15 mL was extracted twice at pH < 1 with ethyl acetate, both fractions were analyzed by LSC (duplicate 1 mL samples)
- ethyl acetate fraction was dried and concentrated, and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- extracted buffer solution of day 15, 22 and 30 were lyophilized followed by acetonitrile extraction; the extract was concentrated and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- duplicate 1 mL ethylene glycol and 10% NaOH trap samples were analyzed by LSC
- silica gel traps were extracted with with methanol, which was then analyzed by LSC; residual radioactivity in the silica traps was determined by combustion
- identity of radioactivity supposed to be CO2 in 10% NaOH trap samples was confirmed for day 22 and 30 by precipitation as BaCO3 and subsequent evolution as CO2 after addition of HCl

On day 30, the reactor was washed with methanol and with acetone. Volumes were measured and 1 mL duplicatealiquots were analyzed by LSC.

Photodegradation was calculated using the SAS Regression Program.

Result : time point (days) 14C-dicamba (% of actually applied

14C-dicamba)*

0	100 (92.14% of applied 14C)
1	98.83
3	95.25
8	86.87
15	75.62
22	66.44
30	58.74 (degradation: 41.26%)
30 (dark control)	98.61

* calculated by reviewer from % of applied 14C
Unchanged dicamba was confirmed by HPLC.

All other compounds in the different fractions, separated by TLC, were <10% of applied 14C and did not match with reference standards. CO2 in the 10% NaOH trap was 11.7% of applied at day 22 and 16.6% of applied 14C at day 30. Radioactivity in the other traps was <10% of applied 14C at all time points. Reactor wash yielded 0.3% of applied activity. The mass balance was >99% and <103.5% at all time points.

Under these conditions, t1/2 of dicamba was 38.1 days; the photolysis rate constant was 0.018 day-1. Based on the spring sunlight intensity at 40 deg latitude at noon (5.83E2 W/m2) the corresponding photodegradation rate for natural sunlight will be 0.0138 day-1; t1/2 will be 50.3 days.

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : I, CAS 1918-00-9 (dicamba), purity 99.6% by IR
I, (14C-dicamba), radiochemical purity 100% by TLC
Conclusion : The photodegradation rate constant in spring sunlight at 40 deg latitude at noon is 0.0138 day-1; t1/2 is 50.3 days. The major photodegradation product is CO2.
Reliability : (1) valid without restriction
1. In the calculation of t1/2, no correction for the degradation in the dark control was made. However, this will only slightly influence the results, as there was hardly any degradation in the dark control.
2. Except for sterilization of the buffer solution, no measures to guarantee sterility of the samples were described. However, as there was hardly any degradation in the dark control (which was a subsample of the sample to be irradiated), it can be assumed biodegradation was negligible.
Flag : Critical study for SIDS endpoint
25.12.2001 (10)

Type : air
Light source : Sun light
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000002985 cm³/(molecule*sec)
Degradation : = % after 43 hour(s)
Deg. product :
Method :
Year : 2001
GLP : no
Test substance :

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

25.12.2001 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Degradation	:	= 0 - 7.6 % after 30 day(s) at pH and °C
Deg. product	:	
Method	:	other: essentially OECD 111
Year	:	1981
GLP	:	no
Test substance	:	

Method : Solutions of 10 ppm and 100 ppm dicamba (1.17% and 0.12% 14C-dicamba, respectively) in distilled water or aqueous buffer solutions of pH 5.0, 7.0 and 9.0 were incubated at 25 and 35 deg C for 30 days (volume 201 mL, in amber bottles in shaking water baths). Acetone concentrations were 0.5%. After 1, 7, 14, 21 and 30 days, a duplicate 1-mL sample was taken for radioassay and a duplicate 15-mL sample was taken for extraction using diethyl ether (at pH < 1). Organic and aqueous layers were first radioassayed and then analyzed using TLC and radioautography detection, followed by quantification using LSC. Samples were cochromatographed with dicamba and three metabolite reference standards.

Result : There was no significant dicamba hydrolysis (i.e. equal to or less than 7.6%) at each pH value, both concentrations and both temperatures, except for 100 ppm, pH 7.0, 35 deg C at t=14, 21 and 30 days in the 100 ppm, when degradation was up to 18.5%. Total recovery was only 82.5-83.4% for these samples, whereas it was > 95 for all other samples. Radioactivity remaining in the aqueous phase after extraction was equal to or less than 1% of applied. Three unknown degradation products each constituted less than 4% of applied.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (14C-dicamba), purity not specified
I, CAS 1918-00-9 (14C-dicamba), radiochemical purity greater than 98%

Conclusion : Dicamba is stable with slight or no hydrolysis over 30 days under the conditions tested.

Reliability : (2) valid with restrictions
1. The fact that at 100 ppm, pH 7.0, 35 deg C up to 18.5% degradation occurred was disregarded because recoveries were low. However, no explanation was given for the low recoveries. It cannot be excluded that loss of radioactivity is due to hydrolysis.
2. Section "Results and discussion" contained 2 values that were not in agreement with values in tables of results.
3. No measures to guarantee sterility of the samples or to exclude oxygen from the solutions were described. However, as measured degradation percentages were very low (except at 100 ppm, pH 7.0, 35 deg C), no significant biotic degradation or oxidation can have occurred.

2. No duplicate samples at any pH.
3. pH 5.0 was tested, whereas OECD 111 prescribes pH 4.

25.12.2001 (19)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air :
Water :
Soil :
Biota :
Soil :
Method :
Year : 2001

Remark : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Measured values were used for physical constants. Biodegradation was based on the current best estimate (from HSDB). Half life in air was determined from the APOWIN program. Direct photolysis was not considered in this model. Other parameters used the default values found in EPIWIN.

Result : Full EPIWIN Output:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Dicamba
  Molecular Wt: 221.04
  Henry's LC  : 2.18e-009 atm-m3/mole (Henry database)
  Vapor Press : 1.26e-005 mm Hg  (user-entered)
  Liquid VP   : 6.95e-005 mm Hg  (super-cooled)
  Melting Pt  : 100 deg C (user-entered)
  Log Kow     : 2.21  (user-entered)
  Soil Koc    : 66.5  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.0498          43           1000
   Water     29.9            500          1000
   Soil      70              500          1000
   Sediment  0.122           2e+003       0

            Fugacity    Reaction    Advection   Reaction    Advection
             (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
 Air       9.61e-013    14.2        8.8         0.473       0.293
 Water     2.6e-014     732         528         24.4        17.6
 Soil      3.58e-013    1.72e+003   0           57.2        0
 Sediment  2.06e-014    0.75        0.0433      0.025       0.00144

   Persistence Time: 590 hr
   Reaction Time:    718 hr
   Advection Time:   3.29e+003 hr
   Percent Reacted:  82.1
   Percent Advected: 17.9

   Half-Lives (hr), (based upon user-entry):
      Air:      43
      Water:    500
      Soil:     500
      Sediment: 2000

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1918-00-9 (dicamba)
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

25.12.2001 (3)

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	
Remark	:	Dicamba has a half life of 31 days with a first-order rate constant of 0.0224/day in a typical midwestern agricultural soil under aerobic conditions. Dicamba is completely mineralized to CO2 under aerobic conditions with 3,6-dichlorosalicylic acid as the only major metabolite. Low levels of 2,3-dihydroxy-3,6-dichlorosalicylic acid were detected. Metabolism under anaerobic conditions is similar to that which occurred in aerobic soil except the rate of dicamba metabolism is reduced under anaerobic conditions. [Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001. AQUATIC FATE: Based on the results of various studies, microbial degradation appears to be the important dicamba removal process in natural water. Photolysis may contribute to dicamba removal from water(Scifres CJ et al; J Environ Qual 2: 306 (1973) As cited in HSDB update of 8-09-2001.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 1918-00-9 (dicamba)
Conclusion	:	Dicamba biodegrades under both aerobic and anaerobic conditions, it is not know if it can be considered readily biodegradable by the OECD criteria.
Flag	:	Critical study for SIDS endpoint

25.12.2001

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Cyprinodon variegatus (Fish, estuary, marine)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> 180
Limit test	:	
Analytical monitoring	:	no
Method	:	other: EPA-660/3-75-00
Year	:	1975
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS
- Species: Cyprinodon variegatus
- Supplier: commercial supplier in Florida
- Size (mean)/weight (mean)/loading: 32 mm/480 mg/0.32 g/L
- Feeding (pretreatment): disontinued 48 hours prior to test
- Feeding during test: none

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: acetone
- Concentration of vehicle/ solvent: 0.06-0.6 mL/L

DILUTION WATER
- Source: artificial seawater (origin well water)
- Chemistry (Salinity;pH): 27 ppt; 8.18

TEST SYSTEM
- Test type: static
- Concentrations: 18, 32, 56, 100 and 180 mg/L, solvent treated and untreated controls
- Exposure vessel type: 20 L glass vessel containing 15 L water
- Number of fish: 10/treatment
- Photoperiod: not indicated

PHYSICAL MEASUREMENTS
- Measuring times: 0, 48 (only O2), 96 h in controls, 18, 56 and 180 mg/L
- Dis. oxygen: 101-104% (0 h), 74-83% (48 h), 51-78% (96 h)
- pH: 7.5-8.2, for 180 mg/L 6.6-7.4
- Test temperature: 21 C

DURATION OF THE TEST: 96 hours

TEST PARAMETER: Mortality
OBSERVATION TIMES: 24, 48 and 96 hours

STATISTICAL METHOD: not applicable

Result : RESULTS:
- Mortality: no mortality
- Other effects: not reported

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (dicamba technical), purity 86.82%
Reliability	:	(2) valid with restrictions Since there is no specific guideline for saltwater fish, the test performance was checked with EPA OPPTS 850.1075 (1996):

A) No analyses were performed to confirm the nominal test concentrations (EPA >80% of nominal)
B) The dissolved oxygen concentration was lower than recommended in some test vessels at the end of the test only (51-78% at 96 hours, EPA >60%); the salinity was higher than recommended (27 ppt, EPA 20 +/- 5 ppt); vehicle concentration was higher than recommended in the highest tested concentration only (0.6 mL/L, EPA 0.5 mL/L); pH-values in the highest tested concentration only were lower than recommended (6.6-7.4, EPA 7.5-8.5), due to inherent properties of the test substance; the photoperiod was not indicated (EPA 12-16 h light).

28.03.2001 (20)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	> 100 measured/nominal
Method	:	
Year	:	1980
GLP	:	no data
Test substance	:	
Method	:	The study was reported in the HSDB record for dicamba as follows: EC50 Daphnia magna greater than 100 mg/l/48 hr @ 21 deg c, first instar /technical material, 88%/. effect: immobilization. static bioassay without aeration, ph 7.2-7.5, water hardness 40-50 mg/l as calcium carbonate and alkalinity of 30-35 mg/l.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 1918-00-9 (dicamba, technical), purity 88%
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

27.12.2001 (17)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: biomass/growth rate
Exposure period	:	120 hour(s)
Unit	:	mg/l
NOEC	:	3.7
EC0	:	3.7
EC10	:	> 3.7
EC50	:	> 3.7
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: EPA 122-2, 123-2
Year	:	1982
GLP	:	yes
Test substance	:	other TS
Method	:	TEST ORGANISMS

- Species: Selenastrum capricornutum, strain 1648, family Chlorophyceae
- Source/supplier: Carolina Biological Supply Company, Burlington, North Carolina
- Laboratory culture: stock culture at Springborn Laboratories
- Culturing: stock cultures were grown in 125 mL glass flasks containing 50 mL test medium and were transferred to fresh medium ~twice weekly.
- Pretreatment: at least 2 days prior to test initiation algae were maintained under test conditions (culture medium, 100 rpm, 25 C, continuous illumination (3200-4300 lux)
- Initial cell concentration: 0.3 E4 cells/mL

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none

GROWTH/TEST MEDIUM CHEMISTRY
- Chemistry (Hardness (Mg+Ca) 0.4 mmol/L;TOC 2.1 mg/L;P 1.6 mg/L;N 14 mg/L;EDTA 12E-2 mmol/L)
- pH: 7.5 (after adjustment)

TEST SYSTEM
- Test type: static
- Concentrations: 4 mg a.i./L and controls
- Exposure vessel: 125 mL erlenmeyer flasks containing 50 mL of test medium (shaken at 100 rpm)
- Number of replicates: 3
- Photoperiod (intensity of irradiation): continuous (3200-4800 lux)

PHYSICAL MEASUREMENTS
- Measuring times: 0 and 120 h
- Test temperature: 25 C
- pH: 7.3-7.5 (0 h); 10.4 (120 h)

DURATION OF TEST: 120 hours

TEST PARAMETER: algal growth (cell counts), measured by a haemacytometer
OBSERVATION TIMES: 0, 24, 48, 72, 96, 120 h

ANALYSES:
- Method: direct HPLC-UV
- Sampling times: 0 and 120 h

STATISTICAL METHOD: t-test

Result **:** RESULTS:
- Nominal concentrations (mg a.i./L): 0, 4
- Measured concentrations (mg a.i./L): <LOQ, 3.7 (=93% of nominal)
- Cell density data after 0, 24, 48, 72, 96 and 120 h (x E4 cells/mL) :
0: 0.3, 3, 18, 39, 54, 258
4: 0.3, 3, 17, 44, 51, 260
- Growth rate/ biomass(AUC) (% of control): 100/99

GROWTH FACTOR CONTROL: 130 after 72 hours

ANALYTICAL RESULTS: validated at 0.025-2.5 mg/L (recovery 101+/-2%, LOQ 14 ug/L. QCs fortified at 4 mg/L showed a recovery of 83-119%.

STATISTICAL RESULTS: no significant differences between control and treatments

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (Dicamba technical), purity 89.5%

Reliability : (1) valid without restriction
Minor remark. The test medium was not in accordance with OECD 201. The pH-increase observed during the test was probably associated with the strong cell growth (factor 130 after 72 hours).

28.03.2001 (9)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1465 mg/kg bw
Species	:	rat
Strain	:	other: Spartan
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: corn oil
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: not specified
- Age: not specified
- Number: 5/sex/dose
- Weight at study initiation: 200-248 g
- Controls: no

ADMINISTRATION:
- Doses: 500, 794, 1250, 1984, 3150 and 5000 mg/kg bw
- Doses per time period: single
- Volume administered: 10 ml/kg bw for all dosage levels except for the 5000 mg/kg level where 20 ml/kg bw was administered.
- Post dose observation period: 14 days
- food was withheld overnight

EXAMINATIONS: for mortality (at least daily).

BODY WEIGHT: at dosing and at 14 days.

STATISTICAL METHOD: Thompson (1947)

Result :

MORTALITY:
- Number of deaths at each dose: 500, 794, 1250, 1984, 3150, 5000 mg/kg bw
0/10, 1/10, 4/10, 4/10, 10/10, 10/10
- Time of death: within 48 hours after dosing

CLINICAL SIGNS: no data on decendents

BODY WEIGHT: all surviving rats exhibited normal body weight gains during the observation period

NECROPSY FINDINGS: no data

POTENTIAL TARGET ORGANS: no data

SEX-SPECIFIC DIFFERENCES:
LD50 males= 1879 mg/kg bw
LD50 females= 1581 mg/kg bw

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (Dicamba 85.8%), purity 85.8%
Conclusion	:	LD50 1707 mg/kg bw = 1465 mg a.i./kg bw
Reliability	:	(2) valid with restrictions

1. The information was essentially confined to what is included in the current summary.
2. no data were presented for effects other than mortality.
3. The dose volume used at the 5000 mg/kg bw was higher than recommended (20 ml/kg, OECD 401 =< 10 ml/kg). Since at 3150 mg/kg all rats died already, the reliability is not lowered because of this.

04.04.2001 (18)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 8.2 mg/l
Species	:	rat
Strain	:	other: Spartan
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: no vehicle
Doses	:	
Exposure time	:	4 hour(s)
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: not specified
- Age: not specified
- Weight at study initiation: 206-245 g
- Number of animals: 5/sex/dose
- Controls: no

ADMINISTRATION:
- Type of exposure: whole body exposure to dust of test material
- Exposure duration: 4 hours
- Concentrations(nominal/measured): approx. nominal conc. of 9.6 mg/l or 8.2 mg a.i./l
- Particle size: not specified
- Type or preparation of particles: control by Wright Dust Feeder
- Air changes: no data

EXAMINATIONS: during exposure: changes in behavior and appearance, after exposure: pharmacodynamic and/or toxic signs; 14 days observation period

BODY WEIGHTS: not specified

ANALYSES:
- Method: no data
- Sampling times: no data

STATISTICAL METHOD: no data

Result :

MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: during exposure: increased, then decreased motor activity, and nasal porphyrin discharge. 14 day observation period decreased motor activity (1/10), corneal

opacity (few rats).

BODY WEIGHTS: gains were normal during the study.

NECROPSY FINDINGS: no data

POTENTIAL TARGET ORGANS: no data

SEX-SPECIFIC DIFFERENCES: no data

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ
Test substance : I, CAS 1918-00-9 (Dicamba 85.8%), purity 85.8%
Conclusion : LC50 > 9.6 mg/l = > 8.2 mg a.i./l
Reliability : (2) valid with restrictions
1. The information was essentially confined to what is included in the current summary
2. As this is a limit test, the LC50 value was derived by the reviewer.
3. no individual data were present.

04.04.2001 (18)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > 1716 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 4
Vehicle : other: not specified
Doses :
Method : other: not specified
Year :
GLP : no
Test substance : other TS

Method : TEST ORGANISMS:
- Source: not specified
- Age: not specified
- Weight at study initiation: 2324-2454 g
- Controls: no

ADMINISTRATION:
- Area covered: not specified
- Occlusion: yes
- Vehicle: not specified
- Concentration in vehicle: not specified
- Total volume applied: not specified
- Doses: 2000 mg/kg bw
- Removal of test substance: washed with tepid tap water after 24 hours

EXAMINATIONS: observed for mortality over 14 days.

BODY WEIGHT: pre-dosing and at day 14

STATISTICAL METHOD: not specified

Result : MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: not specified

BODY WEIGHTS: normal gains during study period

NECROPSY FINDINGS: no data

POTENTIAL TARGET ORGANS: no data

SEX-SPECIFIC DIFFERENCES: no data

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1918-00-9 (Dicamba 85.8%), purity 85.8%
Conclusion	:	LD50 > 2000 mg/kg bw = > 1716 mg a.i./kg bw
Reliability	:	(4) not assignable 1. The information was essentially confined to what is included in the current summary. 2. As this is a limit test, the LD50 value was derived by the reviewer. 3. Only 4 animals were used (OECD 402 5) of which 2 had an abraded skin, which could alter the permeability of the test substance. 4. no individual data were present.

04.04.2001 (18)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	other: CD
Route of admin.	:	oral feed
Exposure period	:	21 weeks
Frequency of treatm.	:	
Post exposure period	:	none
Doses	:	1000, 5000 and 10000 ppm
Control group	:	yes
NOAEL	:	= 342 mg/kg bw
Method	:	EPA OPP 82-1
Year	:	1978
GLP	:	yes
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Species: Charles River CD rat
- Source: Charles River Laboratories, Portage, Michigan
- Age: exact age was not mentioned
- Weight at study initiation: male (122-164 g) female (111-145 g)
- Number of animals: 20/sex/dose group

ADMINISTRATION / EXPOSURE
- Exposure period: 21 days
- Route of administration: diet
- Post exposure period: none
- Doses: 1000, 5000 and 10000ppm, resulting in 69.4, 342 and 682 mg/kg bw/day for males and 79.5, 392 and 751 mg/kg

bw/day for females

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality/clinical signs: twice daily, detailed observations weekly
- Body weight: weekly
- Individueal food consumption: weekly

CLINICAL LABORATORY TESTS
In 10 rats/sex/dose group at baseline and in week 6 and 13.
- Haematology: hemoglobin, hematocrit, erythrocyte count, yotal and differential leukocyte counts, platelet count, mean corpuscular volume (MCV), mean corpuscular hemoglobin (MCH), mean corpuscular hemoglobin concentrations (MCHC), and reticulocyte count.
- Biochemistry: sodium, potassium, chloride, alkaline phosphatase, blood urea nitrogen (BUN), serum glutamic pyruvate transaminase (SGPT), serum glutamic oxaloacetate transaminase (SGOT), calcium, creatinine, phosphorous, lactic dehydrogenase (LDH), glucose, total bilirubin total cholesterol, albumin, globulin, total protein.
- Urinalysis: specific gravity, volume, color and appearance, occult blood, protein, pH, bilirubin, urobilinogen, ketones, glucose, microscopic examination sediment, nitrites, urobilinogen, ketones.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: brain, heart, kidneys, liver, gonads,
- Microscopic (control animals and 10000 ppm, heart, liver, kidneys and gross lesions in all groups): all gross lesions, adrenals, eye, trachea, esophagus, stomach, duodenum, jejenum, ileum, caecum, colon, liver (2 sections), spleen, urinary bladder, testes/ ovaries, pancreas, brain (3levels-forebrain, midbrain, hindbrain), heart, lungs+mainstem bronchi, pituitary, thyroid and parathyroid, thymus, lymph node (mesenteric), sternum (bone marrow), spinal cord), salivary gland, (submaxillary), skeletal muscle (thigh), kidneys, prostate/ corpus and cervix uteri, peripheral nerve (sciatic).

ANALYSES:
- homogeneity of diet before study inititation
- stability of test article at weeks 1,3,4,8 and 13 by GC/ECD

STATISTICAL METHODS:
- analyses of variance, Bartlett and t-test as described by Steel and Torrie

Result : CLINICAL SIGNS/MORTALITY
- Mortality (dweek): 1 female control (6), 1 female 5000 ppm (2), 1 female 10000 ppm (13); Three female rats died during the course of the study.

- Clinical signs: No changes were seen in general behavior and appearance;
incidental findings in treated rats: rales, yellow material on the anogenital region, mouth ulcer, pale exposed skin areas, black material on or around the eye, nose, mouth or anogenital region, corneal opacity, dilated pupil, eye enlarged and protruded, increased distance between pupil and cornea, nose malaligned, swollen foot, portion of the ear

missing, and portion of the tail black or missing. These signs were noted randomly among the treated rats.
One mid-dose male rat had a subcutaneous mass in the anogenital region.
Incidental findings in both treated and control rats: malaligned upper incisors, red areas around the eyes, scabbing, excessive lacrimation and hair loss.

- Body weight gain: slightly decreased at 10000 ppm in both sexes, significantly in week 13.

- Food consumption: at 10000 ppm decreased consumption in both sexes

CLINICAL CHEMISTRY
- hematology: no abnormalities; one female at 10000 ppm had elevated leucocyte, reticulocyte and platelet counts and slightly decreased hemoglobin, hematocrit and erythrocyte count
- Biochemistry: slightly elevated ALP activity at 10000 ppm (weeks 6 and 13) significance at group means level; at week 13 (2 males at 5000 and 2 females and 1 male at 10000 ppm) decreased glucose in both sexes at 5000 and 10000 ppm (but within biological range) significance at group means level
- Urinalysis: no abnormalities

MACRO- AND MICROSCOPIC FINDINGS:
No gross leasion were seen.
- Organ weights: no treatment related variations
- Histopathology: absence or reduction in cytoplasmic vacuolation in hepatocytes at all dose levels (and so a reduction of liver glycogen)

ANALYSES:
- stability of test substance: after 7 day storage values ranged from 79-87% of target concentration, samples taken in week 1-4, 8 and 13 had mean concentrations of 84, 96 and 83% of target concentration for 1000, 5000 and 10000 ppm respectively.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1819-00-9 (2-methoxy-3,6-dichlorobenzoic acid), purity 86.8%
Conclusion : NOAEL 342 mg/kg bw based on effects on body weight, food consumption and elavated ALP
Reliability : (1) valid without restriction
21.05.2001 (6)

Type :
Species : rabbit
Sex : male/female
Strain : New Zealand white
Route of admin. : dermal
Exposure period : 3 weeks
Frequency of treatm. : 5 days a week
Post exposure period : none
Doses : 100, 500, 2500
Control group : yes
Method :
Year :
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS:
- Species: New Zealand white rabbits
- Age: no data
- Weight at study initiation: males: 1.9 - 2.6 kg, females: 2.1-2.7 kg
- Number of animals: 4/sex/dose group

ADMINISTRATION / EXPOSURE
- Doses: 100, 500 and 2500 mg/kg/day
- Exposure period: 21 days
- Duration of exposure: 6 hours
- Route of administration: dermal
- Post exposure period: none
- Vehicle: 0.9% saline
- Total volume applied: no details given. Maximum vehicle amount used was 5ml.
- Area exposed: 10% of body surface
- Occlusion: not specified
- Removal of test substance: by wiping

CLINICAL OBSERVATIONS AND FREQUENCY:
- pre- and post-test determination of hematological and biochemical blood parameters (total and differential leukocyte counts, erythrocyte count, hematocrit, hemoglobin, alkaline phosphatase, blood urea nitrogen, glutamic pyruvate transaminase, glutamic oxaloacetate transaminase, calcium, inorganic phosphorus, fasting blood glucose, albumin, total protein)
- pre- and post-test urinalysis (volume, specific gravity, color and appearance, pH, albumin, glucose, occult blood and billirubin)
- Clinical signs and mortality: daily observations, scoring of dermal irritation
- Body weight: weekly

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: The spleen, liver, adrenals, ovaries/ testes, thyroid (parathyroid), brain and kidneys were weighed fresh.
- Microscopic: skin (treated and untreated), gallbladder, lung, trachea, liver, kidneys, large intestine, small intestine, stomach, pancreas, urinary bladder, spleen, heart, regional lymph node, mesenteric lymph node, prostate/uterus, testes/ovaries, pituitary, thymus, thyroid/pars, adrenals, thyroid, eye, nerve, muscle, bone marrow, spinal cord, brain, any unusual lesions

STATISTICAL METHODS:
analysis of variance (one-way classification), Bartlett's test, Dunnett's multiple comparison tables

Result : TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time of death: males: 1(9) control, 1(17) 100 mg/kg; females 1(18) 100 mg/kg, 2(6&10) 500 mg/kg, 2(6&7) 2500 mg/kg

- Clinical signs:
Animals that died: diarrhea, hypoactivity, distended abdomen, anorexia and slight cyanosis.
Surviving animals diarrhea and soft stools, erythema, desquamation, atonia, coriaceousness, fissuring

- Body weight gain: no abnormalities

- Clinical chemistry: blood glucose in females at 2500 mg/kg significantly higher than controls, but within biological range

- Haematology: no abnormalities

- Urinalysis: Significant difference in pH for males at 2500 and females at 100 mg/kg compared to controls, but values were within biological range

NECROPSY FINDINGS
- Organ weights: increased adrenal weight (not toxicologically significant)

- Gross pathology:
skin thickening and erythema of the application site in 2 rabbits at 2500 mg/kg/day

- Histopathology: at application site: acanthotic epidermal thickening and hyperkeratosis, slight parakeratosis. No dose response

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9, (2-methoxy-3,6,-dichlorobenzoic acid), purity 86.8%

Reliability : (3) invalid
1. Too many animals died. From 8 control and 24 dosed rabbits one control and 6 exposed rabbits died during the study.
2. Five of the six animals that died were female rabbits. Therefore 43% of the dosed female rats did not survive the study. This was not considered in the discussion of the data.
3. The purity, stability and composition of the compound were not determined.
4. The food consumption was not monitored.

21.05.2001 (7)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : TA98, TA100, TA1535, TA1537 and TA102
Test concentration : 8-5000 ug/plate
Cycotoxic concentr. : 1500 ug/plate
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1983
GLP : yes
Test substance : other TS

Method : SYSTEM OF TESTING:
- Species/cell type: Salmonella typhimurium TA98, TA100, TA1535, TA1537 and TA102.
- Deficiences/Proficiences: histidine-requiring strains
- Metabolic activation system: rat S-9 mix, Arochlor 1254 induced

ADMINISTRATION:
- Dosing:
Mutation experiment 1 (without preincubation): 8, 40, 200, 1000, 5000µg/plate;
Mutation experiment 2: TA98, TA100, TA1535, and TA1537: 187.5, 375, 750, 1500 and 3000 ug/plate. TA102: 46.875, 93.75, 187.5, 375 and 750µg/plate.
- Number of replicates: 3
- Application: solution in DMSO
- Positive and negative control groups and treatment:
Positive controls: -S9: 2-nitrofluorene (TA98), sodium azide (TA100, TA1535), 9-aminoacridine (TA1537), gluturaldehyde (TA102).
+S9: 2-aminoanthracene (at least one strain).
Negative controls: DMSO (vehicle)
- Pre-incubation time: Mutation experiment 2; 1h incubation at 37°C of S9 with the test compound prior to addition to the tester strain.

CRITERIA FOR EVALUATING RESULTS:
- Statistical method: Dunnett's test
- Method of calculation: linear regression analysis

Result : GENOTOXIC EFFECTS:
- With metabolic activation: none
- Without metabolic activation: none
PRECIPITATION CONCENTRATION: no precipitation was observed
CYTOTOXIC CONCENTRATION: 1500 ug/plate with and without metabolic activation

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9 (3,6-dichloro-2-methoxybenzoic acid), purity 88.5%

Reliability : (1) valid without restriction
16.05.2001 (2)

Type : Chromosomal aberration test
System of testing : CHO cells
Test concentration : 300-2330 ug/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : yes
Test substance : other TS

Method : - Species/cell type: Chinese hamster ovary (CHO-K1) cells
- Metabolic activation system: rat S9 mix (Aroclor 1254 induced)
- No. of metaphases analyzed: 100

ADMINISTRATION:
- Dosing: 2330, 1170, 590 and 300 µg/ml.
- Number of replicates: 2
- Application: solution in DMSO
- Exposure time: 8 hours (-S9) or 2 hours (+S9)
- Clocemid at final concentration of 10 ug/mL.
- Positive and negative control groups and treatment:
Positive controls: with S-9: triethylene melamine; without S-9: cyclophophamide
Negative controls: DMSO

CRITERIA FOR EVALUATING RESULTS:
- Statistical method: Student's t test
- method of calculation: linear regression analysis

Result : GENOTOXIC EFFECTS:
- With metabolic activation: none
- Without metabolic activation: none

PRECIPITATION CONCENTRATION: No precipitation was observed

CYTOTOXIC CONCENTRATION: No cytotoxicity was observed

STATISTICAL RESULTS: no significant increase in number of aberrations in test group compared to control group.

Positive control triethylene melamine gave 0.45 structural aberrations per cell, positive control Cyclophosphamide induced 0.69 aberrations per cell. This was in both cases a significant increase above the untreated control

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9, (3,6-dichloro-2-methoxybenzoic acid), purity 88.5%

Reliability : (2) valid with restrictions
1. Only 100 metafases are scored (OECD 473: at least 200)

21.02.2003 (8)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay
Species : mouse
Sex :
Strain : ICR
Route of admin. : i.p.
Exposure period : single dose
Doses : 450, 900 and 1800 mg/kg bw
Result : negative
Method :
Year :
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS:
- Species: ICR mice
- Source: Harlan Sprague Dawley Inc., Frederick, MD.
- Age: 6 to 8 weeks
- Weight at study initiation: males (29.5 - 36.6g), females (25.5 - 32.0g)
- No. of animals per dose: 15/sex/dose

ADMINISTRATION:
- Vehicle: deionized distilled water
- Doses: 0, 450, 900, 1800 mg/kg bw.
- Duration of test: Five animals of each dose group were killed after 24, 48, and 72 hr dosing.
- Frequency of treatment: single dose by i.p. injection
- Sampling times and number of samples: 24, 48 and 72 hours; 2-4 slides per animal
- Control groups and treatment:
Negative control group: vehicle 15 animals per sex.

Positive control: cyclophosphamide, 5 animals per sex.

EXAMINATIONS:
- mortality and clinical signs
- number of micronucleated Polychromatic erythrocytes (PCE)/1000 PCE
- number of PCE/total erythrocyte (1000 erythrocytes scored)

Evaluation of Test Results:
statistical: Kastenbaum-Bowman

Remark : The DMA salt of dicamba is the test substance.

Result : Mortality: males 4/20 and 1/15, females 3/20 and 0/15 at 1800 and 900 mg/kg resp.

Clinical signs: lethargy at all dose levels

EFFECT ON PCE/NCE RATIO:
- number of micronucleated PCE per 1000 PCE:
450 mg/kg bw: 0.8, 0.3 and 0.2 at 24, 48 and 72 hours resp.
900 mg/kg bw: 0.9, 0.1 and 0.2 at 24, 48 and 72 hours resp.
1800 mg/kg bw: 1.4, 0.6 and 0.3 at 24, 48 and 72 hours resp.
- PCE/total erythrocytes
450 mg/kg bw: 0.65, 0.60 and 0.56 at 24, 48 and 72 hours resp.
900 mg/kg bw: 0.60, 0.58 and 0.56 at 24, 48 and 72 hours resp.
1800 mg/kg bw: 0.59, 0.52 and 0.62 at 24, 48 and 72 hours resp.

Statistical results:
micronucleated PCE/1000 PCE was not significantly increased at any dose level at any collection time in either males or females.
The positive control induced a significant increase in micronucleated PCE/1000 PCE

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : Dicamba DMA salt, purity 40.3%

Reliability : (3) invalid
1. Purity of the test substance is unknown. It is not mentioned what DMA (DMA salt of dicamba) stands for.
2. Only 1000 erythrocytes are scored for incidence of micronucleated PCE (OECD 474, 1997: at least 2000)
3. Sampling at 72 hours is too late. However 2 sampling times remain (24 and 48 hours), which is sufficient according to OECD 474, 1997.

21.05.2001 (11)

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study

Species : rat

Sex : male/female

Strain : other: Crl:CD-(SD) BR VAF/Plus

Route of admin. : oral feed

Exposure period : Parent-generation (males/females): 10 weeks prior to mating until weaning of the litters (day 21 post-partum); F1-generation 12 weeks prior to mating until weaning of the litters (day 21 post-partum)

Frequency of treatm. : continuous

Premating exposure period

Male	:	10 weeks (parental generation) or 12 weeks (F1-generation)
Female	:	10 weeks (parental generation) or 12 weeks (F1-generation)
Duration of test	:	50 weeks
No. of generation studies	:	
Doses	:	500, 1500 and 5000 ppm in the diet
Control group	:	other: diet without the test substance
NOAEL parental	:	= 1500 ppm
NOAEL F1 offspring	:	= 1500 ppm
NOAEL F2 offspring	:	= 500 ppm
Method	:	OECD Guide-line 416 "Two-generation Reproduction Toxicity Study"
Year	:	1983
GLP	:	yes
Test substance	:	other TS

Method :

TEST ORGANISMS (PARENTAL GENERATION):
- Age: males/females 6 weeks at start treatment
- Weight at study initiation: At start treatment males 180-271g and females 137-190g
- Source: Charles River UK Ltd
- Number of animals: 32/sex/treatment (parental), 28/sex/treatment (F1)

ADMINISTRATION / EXPOSURE
- Test duration: maximum 50 weeks
- Exposure period: males and females 10 weeks (parent generation) or 12 weeks (F1-generation) prior to mating and until weaning of the F1 or F2 generation, respectively
- Route of administration: oral via the diet
- Doses: 0, 500, 1500 and 5000 ppm in the diet

MATING PROCEDURES (PARENTAL AND F1-GENERATION):
- Mating: 1 female / 1 male (or occasionally 2 females / 1 male) during 20 days
- Day 0 of gestation: presence of vaginal plugs and/or spermatozoa in the vaginal smear of females

PARAMETERS ASSESSED DURING STUDY (PARENTAL AND F1-GENERATION):

- Mortality/clinical observations: regularly
- Body weight gain: weekly (males/females) or daily for females during mating and until parturition
- Food consumption: weekly during the premating treatment phases
- Water consumption: daily during initial and final two weeks of the premating treatment periods
- Female oestrous cycle: vaginal cytology examination 7 days prior to mating (parental generation) and the first mate of the F1-generation and during the 20-day mating period
- Male sperm analysis: at necropsy samples from both vas deferens were analysed for total count, motility and morphology (1 every 4 male rat/cage). Left testis examined for spermatid counts
- Mating and fertility data (males/females): number and days of successful matings, time between pairing and mating (with 1rst or 2nd male, F1-generation)
- Maternal delivery data: duration of gestation, number pregnant, litter size (live pups) and number of implant sites
- Pup viability: number of live pups at birth and post-partum days 4, 8, 12, 16, 21 (culling on day 4

post-partum to 8 pups/litter)
- Pup observations: clinical signs, sex and external examinations; body weights on days 1 (birth), 4, 8, 12, 16 and 21 post-partum; sexual maturation of female pups by the unset of vaginal opening (as of day 28 post-partum) and of males pups by the occurrence of cleavage of the balanopreputial skinfold (as of day 35 post-partum)

ORGANS EXAMINED AT NECROPSY (PARENTAL AND F1-GENERATIONS):
- Macroscopy: all males and females (parental generation), those selected for pairing (F1-generation) and one male and one female pup from each litter (day 21 post-partum) were necropsied and gross findings recorded. The following organs were weighed; adrenals. brain, heart, kidneys, liver, lungs, pituitary prostate (with seminal vesicles and coagulating gland) tests with epididymides and thymus. Additionally, a full range of tissues (see microscopy) was preserved for histopathology.
Remaining pups were examined externally and internally and the sex was confirmed by gonadal inspection. Gross findings were preserved (when considered usefull) for possible histopathology
- Microscopy: histopathology examinations were preformed on the adrenals, aorta, bone and joint, bone marrow, brain, cranial vault, caecum, colon, duodenum, eyes, heart, ileum, jejunum, kidneys, liver, lungs, lymph nodes, mammary gland, oesophagus, ovaries, pancreas, pituitary, prostate (for F1 weanlings with seminal vesicles and coagulating gland), rectum, salivary gland, seminal vesicles (with coagulating gland) sciatic nerve, skeletal muscle, skin, spinal column, spleen, stomach, testes, epididymides, thymus, thyroids (with parathyroids), tongue, trachea (with larynx and pharynx), urinary bladderuterus (with cervix) vagina and vas deference

ANALYSES:
- Method: High Performance Liquid Chromatography (HPLC) with UV detection
- Sampling time: prior to start of the first premating treatment (500 ppm and 12000 ppm dietary inclusion levels) for analysis of stability and homogeneity. Samples for accuracy of exposure concentrations for each generation were taken at start of the premating treatment and at start of the mating and end of gestation/start lactation

STATISTICAL METHODS: analysis of variance, Williams' test, Kruskal-Wallis test, Analysis of covariance, Shirley's test, Fisher's exact test

Result : ANALYSES:
- Actual dose level: the accuracy of all test diets was acceptable (94-112% of nominal)
- Stability: stable for at least 18 days (within 91-93%)
- Homogeneity: homogeneous (all samples 91-99% of nominal)
- Actual intake during week 1-10 at 500, 1500 and 5000 ppm:
F0: males 35, 105 and 347 mg/kg bw resp., females 41, 125 and 390 mg/kg bw resp.
F1: males 40, 121 and 432 mg/kg bw resp., females 44, 135 and 458 mg/kg bw resp.

TOXIC EFFECTS BY DOSE LEVEL

PARENTAL GENERATION:

- Mortality: at 500 and 5000 ppm one female
- Body weight gain: at 5000 ppm decreased in females during pregnancy and the first week of lactation
- Food consumption/water consumption: no treatment-related findings
- Clinical signs: incidental hairless and scabbing, but no treatment-related findings
- Mating and fertility data (males/females): no differences between the dose groups (sperm motility, morphology and number normal); pregnant females at 500, 1500 and 5000 ppm 27, 28, 29 and 27 resp.
- Maternal delivery data: at 5000 ppm slight shift of the duration of pregnancy from 22/23 to 21 days and decreased litter and pup weights
- Macroscopic examinations: pale subpleural foci on the lungs of males at 5000 ppm (parent); increased incidence of pelvic dilations in pups (without relationship to dose)
- Organ weights:
parents: at 5000 ppm increased rel. liver weights in females, decreased epididymides, prostate and rel. kidney weight in males; at all treatments decreased pituitary weight (rel.)
pups: at 1500 ppm increased liver and decreased lung weights (both relative); at 5000 ppm decreased absolute brain weight and relative heart and lung and increased relative liver weight
- Microscopic examinations: no treatment-related findings
- Pup viability/observations: at 5000 ppm decreased pup weights and delayed sexual maturation of the males, no effects on sex ratio.

F1 GENERATION:

- Mortality: at 0, 500, 1500 and 5000 ppm, 2 males/1 female, 1 male/1 female, 1 male and 1 male, respectively
- Body weight: decreased in males at 5000 ppm and females at 5000 ppm during the first weeks after weaning
- Food consumption/water consumption: at 5000 ppm in males and females decreased (food weeks 5-8/water weeks 5-6 of premating treatment)
- Clinical signs: at 5000 ppm increased incidence of tense/stiff body tone and slow righting reflex at the latter part of lactation
- Mating and fertility data (males/females): first mate gave pregnancy rate of 56-75%; second mate 56-68%; sperm motility, morphology and number normal
- Maternal delivery data: at 5000 ppm decreased pregnancy rate (first mate), decreased litter weights; slightly higher pup loss (second mate) resulting in slightly lower litter sizes at 1500 and 5000 ppm
- Macroscopic examinations: dose related increase of the number of pale foci on the lungs in parents
- Organ weights:
parents: at 5000 ppm increased liver weights (absolute females, relative males); at all treatments kidney weight decreased relative to body weight
pups: at 5000 ppm increased relative liver weight, decreased rel. kidney and heart weight
- Microscopic examinations: no treatment-related findings
- Pup viability/observations: at 5000 ppm decreased pup

weights and associated delayed male and female sexual maturation

F2 GENERATION:

- Clinical signs: no treatment-related findings
- Pup viability/observations: at 1500 slightly decreased pup weights and at 5000 ppm decreased pup weights and increased liver weights

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (dicamba technical, 3,6-dichloro-o-anisic acid), purity 86.9%

Conclusion : NO(A)EL (parents): 1500 ppm, based on decreased female body weight gain during pregnancy and increased liver weights in both sexes in the 5000 ppm group.
NO(A)EL (F1-generation): 1500 ppm, based on a marked impairment of growth of the F1-offspring and associated reduced food and water consumption, slightly delayed sexual maturation of males and increased liver weights.
Additionally F1-females showed slightly lower body weight gain during pregnancy and signs of increased bodytone and slow righting reflex during late lactation
NO(A)EL (F2 generation): 500 ppm, based on reduced body weight gain of F1-females during pregnancy and slghtly reduced growth of F2-pups

Reliability : (1) valid without restriction
21.02.2003 (5)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Crj: CD(SD)
Route of admin. : gavage
Exposure period : gestation days 6-19
Frequency of treatm. : Once daily
Duration of test : Caesarean sections on gestation day 20
Doses : 64, 160 and 400 mg/kg/day
Control group : yes, concurrent vehicle
NOAEL maternal tox. : <= 160 mg/kg bw
NOAEL teratogen. : <= 400 mg/kg bw
NOAEL Fetotoxicity : <= 400 mg/kg bw
Method : other: US 43 FR 37336, Part 163.83-3
Year : 1981
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS
- Age: females not indicated (sexually mature)
- Weight at study initiation: 196-251g (gestation day 0)
- Number of animals: 25 (treatment/control groups)
- Source: Stone Ridge, N.Y. facilities of Charles River, Breeding Laboratories, Inc. USA

ADMINISTRATION / EXPOSURE
- Test duration: 20 days
- Exposure period: gestation days 6-19
- Route of administration: oral gavage
- Doses: 0, 64, 160 and 400 mg/kg

- Vehicle: corn oil

MATING PROCEDURES:
- Mating: 1 female / 1 male
- Day 0 of gestation: presence of copulation plug and/or sperm in the vaginal smear

PARAMETERS ASSESSED DURING STUDY:
- Mortality: twice daily
- Clinical observations: twice daily (early morning, late afternoon)
- Body weight gain: gestation days 0, 6 and 20
- Food consumption: daily (gestation days 0-19)
- Examination of uterine content: number and distribution of implantations, early and late resorptions and live and dead foetuses
- Examination of fetuses: sex; weight; external, visceral (1/3) and skeletal (2/3 foetuses) findings

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopy: not indicated
- Microscopy: no tissues retained

OTHER EXAMINATIONS:

No

ANALYSES:
- Method: Liquid Chromatograph (HPLC)
- Sampling time: samples taken from all preparations (1 interval subjected to analysis)

STATISTICAL METHODS: Scheffe's or Turkey's

Result : ANALYSES:
- Actual dose level: dose preparations were confirmed to be accurate
- Stability: Stable during at least 1 week

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:

- Mortality and day of death: at 400 mg/kg 3 females died on gestation days 7 or 8
- Body weight: at 400 mg/kg decreased on gestation day 20
- Food consumption: at 400 mg/kg decreased during exposure (gestation days 6-19)
- Clinical signs: at 400 mg/kg females showed increased incidence of crusty nose/muzzle, wheezing, ataxia, stiffening of the body when held, urine soaked fur, salivation and decreased motor activity
- Number pregnant per dose level: at 0, 64, 160 and 400 mg/kg, 23, 24, 23 and 17, respectively
- Number aborting: none
- Number of resorptions (early/late): at 0, 64, 160 and 400 mg/kg, 6.4%, 3.0%, 5.3% and 8.7%, respectively (percent of implantation sites)
- Number of implantations: at 0, 64, 160 and 400 mg/kg, 14.2, 12.3, 14.3 and 13.1, respectively
- Post implantation loss: idem number of resorptions
- Number of corpora lutea: not recorded
- Duration of Pregnancy: scheduled sacrifice on gestation

day 20
- Gross pathology incidence and severity: no findings

FETAL DATA:

There were no gross external, soft tissue or skeletal alterations that were considered effects of the test substance. Foetal body weight and sex were comparable between all groups

- Litter weights (gravid uterus): at 0, 64, 160 and 400 mg/kg, 73g, 66g, 75g and 62g, respectively
- Number viable: at 0, 64, 160 and 400 mg/kg, 13.3, 11.9, 13.6 and 11.8, respectively
- Sex ratio (percentage of males): at 0, 64, 160 and 400 mg/kg, 49.2%, 49.0%, 49.5% and 52.0%, respectively
- Body weight: at 0, 64, 160 and 400 mg/kg, for males 3.5g, 3.5g, 3.4g and 3.3g, respectively and for females 3.3g, 3.3g, 3.2g and 3.1g, respectively.
- Grossly visible abnormalities: at 160 mg/kg one foetus showed a shortened body and anurous
- Visceral abnormalities: at 400 mg/kg increased incidence renal pelvic cavitation (one litter)
- Skeletal abnormalities: at 400 mg/kg one foetus with incomplete frontal(s) and/or parietal(s) ossification

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, CAS 1918-00-9 (dicamba technical, 3,6-dichloro-o-anisic acid), purity 86.9%
I, CAS 1918-00-9 (technical Dicamba), purity: technical grade

Conclusion : NOAEL (maternal): 160 mg/kg based on decreased body weights and food consumption and clinical symptoms such as ataxia stiffening of the body when held and decreased motor activity at 400 mg/kg
NOAEL (teratogenicity): 400 mg/kg based on the absence of any significantly increased malformation or variation
NOAEL (foetotoxicity): 400 mg/kg based on the absence of any effects on foetal growth or deaths

Reliability : (1) valid without restriction
No corpora lutea recorded
Post implantation loss not calculated

21.02.2003 (16)

Species : rabbit
Sex : female
Strain : New Zealand white
Route of admin. : other: oral via capsules
Exposure period : gestation days 6-18
Frequency of treatm. : Once daily
Duration of test : Caesarean sections on gestation day 29
Doses : 30, 50 and 300 mg/kg
Control group : yes, concurrent vehicle
NOAEL maternal tox. : <= 30 mg/kg bw
NOAEL teratogen. : <= 300 mg/kg bw
Method :
Year : 1984
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS
- Age: females (at insemination) 26 weeks

- Weight at study initiation: 3.05-4.14 kg
- Number of animals: 20 (treatment groups), 19 (control group
- Source: Hazelton Research Products, Inc., Denver Pennsylvania, USA

ADMINISTRATION / EXPOSURE
- Test duration: 29 days
- Exposure period: gestation days 6-18
- Route of administration: oral (via capsules)
- Doses: 0, 30, 150 and 300 mg/kg
- Vehicle: opaque white gelatin capsules

MATING PROCEDURES:
- Artificial insemination: Semen collected from 4 proven donor bucks of the same strain and source as the females. 3 hours before insemination females were intravenously injected with 20 USP units of Human Chorionic Gonadotropin. Insemination of 0.25 mL of diluted (with saline) semen sample (6.0 million spermatozoa/0.25 mL)
- Day 0 of gestation: day of insemination

PARAMETERS ASSESSED DURING STUDY:
- Mortality: twice daily
- Clinical observations: once daily or on gestation days 6-19 immediately before dosage and within 60 minutes after dosage
- Body weight gain: once weekly before insemination and on gestation days 0 and 6-29
- Food consumption: daily
- Examination of uterine content: number of corpora lutea; number and distribution of implantations, early and late resorptions and live and dead foetuses
- Examination of fetuses: sex; weight; external, visceral (all foetuses) and skeletal (all foetuses) findings; brains free-hand cross-sectioned and examined for hydrocephaly

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopy: findings all dams recorded, all gross lesions (except commonly found parovarian cysts) were fixed for possible histopathology
- Microscopy: not performed

OTHER EXAMINATIONS:
- Uterus staining: uteri from non-pregnant rabbits were stained with 10% ammonium sulfide to comfirm absence of implantation sites

ANALYSES:
- Method: Not indicated (samples not analysed)
- Sampling time: Bulk test substance sampled on day 2 and the end of the dosing period for possible analysis

STATISTICAL METHODS: Bartlett's Test, Dunnett's Test, Kruskal-Wallis Test, Dunn's Test and Fisher's Exact Test

Result **:** ANALYSES:
- No analyses performed. Test substance dosed via capsules. Data on the identity, composition, strength, purity and stability of the test substance are kept on file with the sponsor

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:

There were no differences noted among the dose groups in the number of corpora lutea, implantations, litter sizes, early and late resorptions, foetal sex ratio, foetal body weights, percent resorbed conceptuses and number of does with any resorptions

- Mortality and day of death: One female dosed at 300 mg/kg died due to an intubation error on gestation day 12. Abortion and subsequent sacrifice occurred in the 150 mg/kg dose group for 1 female on gestation day 22 and in the 300 mg/kg dose group for four females on gestation days 19 (one female), 21 (one female) and 24 (two females)
- Body weight: at 300 mg/kg body weight loss on gestation days 6-7, 6-9, 9-12, 12-15, 15-19 and overall loss during gestation days 6-19. Decreased overall body weight gain during gestation days 6-19 (loss), 6-29 and 0-29
- Food consumption: at 300 mg/kg often during the dosing period resulting in a reduced overall food consumption during gestation days 6-19, 6-29 and 0-29
- Clinical signs: at 150 and 300 mg/kg females showed ataxia (and decreased motor activity). In addition, females receiving 300 mg/kg incidentally showed rales, laboured breathing, perinasal substance (red or yellow), dried faeces, impaired righting reflex, no faeces and a red substance in the cage pan
- Number pregnant per dose level: 16 (80% of number inseminated) in the 30 mg/kg group and 18 in all other groups (90-94.7% of number inseminated)
- Number aborting: at 150 mg/kg 1 and at 300 mg/kg 4
- Number of resorptions (early/late): at 0, 30, 150 and 300 mg/kg, 0.5, 0.5, 1.0 and 0.5, respectively
- Number of implantations: at 0, 30, 150 and 300 mg/kg, 6.8, 5.9, 6.4 and 6.3, respectively
- Post implantation loss: at 0, 30, 150 and 300 mg/kg, 6.4%, 4.8%, 10.1% and 7.6%, respectively
- Number of corpora lutea: at 0, 30, 150 and 300 mg/kg, 9.6, 8.4, 8.9 and 9.2, respectively
- Duration of Pregnancy: scheduled sacrifice on gestation day 29
- Gross pathology incidence and severity: no findings other then those related to intubation error (thick, hard and gray oesophagus and trachea containing white mucoid substance) or commonly found parovarian cysts

FETAL DATA:

There were no gross external, soft tissue or skeletal alterations that were considered effects of the test substance

- Litter size and weights: at 0, 30, 150 and 300 mg/kg, 6.3, 5.4, 5.4 and 5.8, respectively
- Number viable: at 0, 30, 150 and 300 mg/kg, 6.3, 5.4, 5.4 and 5.8, respectively
- Sex ratio (percentage of males): at 0, 30, 150 or 300 mg/kg, 49.4%, 64.4%, 54.7% and 54.6%, respectively
- Body weight: at 0, 30, 150 and 300 mg/kg, 44.55g, 47.11g, 44.20g and 42.47g, respectively
- Grossly visible abnormalities: incidentally observed

findings consisted of umbilical hernia, menigocele, medially rotated hindlimbs, flexed hindpaws and shortened tail
- Visceral abnormalities: incidental findings comprised protrusion of the liver through the abdominal wall, agenesis of the intermediate lobe of the lungs, agenesis of the gall bladder and caudally displaced right kidney.
- Skeletal abnormalities: incidentally observed finding consisted of vertabral malformations (irregular shaped left arch of the 3rd lumbar vertebra and fosion of the left arches of the 3rd and 4th lumbar vertebrae), tail malformation (14 vertebrae present) and variations in skull and sternal ossification (displaced nasal suture, internasal ossification site and fused 3rd and 4th sternebrae)

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : I, 1918-00-9 (Technical dicamba), purity (not reported)

Conclusion : NOAEL (maternal): 30 mg/kg based on the abortions, clinical signs (viz. decreased motor activity, ataxia, rales, laboured breathing, perinasal substance red/yellow, dried faeces, impaired righting reflex, no faeces, red substance in the cage pan), reduced body weight gains and reduced feed consumption
NOAEL (teratogenicity): 300 mg/kg based on the absence of any significantly increased malformation or variation
NOAEL (foetotoxicity): 300 mg/kg based on the absence of any effects on foetal growth or deaths

Reliability : (1) valid without restriction
19.04.2001 (1)

(1) ARGUS RESEARCH LABORATORIES INC, DEVELOPMENTAL TOXICITY (EMBRYO-FETAL TOXICITY AND TERATOGENIC POTENTIAL) STUDY OF TECHNICAL DICAMBA ADMINISTERED ORALLY VIA CAPSULE TO NEW ZEALAND WHITE RABBITS, 1992 (103)

(2) Ballantyne, M., Dicamba Technical: Reverse mutation in five histidine-requiring strains of Salmonella typhimurium

(3) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(4) Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995. 37 (as cited in Hazardous Substance Data Base)

(5) Huntingdon Research Centre Ltd., Huntingdon, England, Technical dicamba A study on the reproductive function of two generations in the rat, 1993

(6) International Research and Development Corporation, 13-week dietary toxicity study in rats with Dicamba, 1980

(7) International Research and Development Corporation, 3-week dermal toxicity study in rabbits, 1979

(8) Microbiological Associates Inc., Chromosome aberrations in Chinese hamster ovary cells, 1986

(9) Sandoz Agro Inc, Dicamba technical - toxicity to the freshwater green alga, Selenastrum capricornutum (BASF 93/5221), 1993 (98)

(10) Sandoz Agro, Dicamba: Photodegradation Study in pH 7 Aqueous Solution (1993) (95) unpublished study

(11) Sandoz Agro, Inc., Micronucleus cytogenetic assay in mice, 1994

(12) Sandoz Agro, Melting Point of Dicamba, Technical (1993) (89)

(13) Sandoz Agro, Solubility of Technical Dicamba in Solvents, unpublished report (1993) (91)

(14) Sandoz Agro, Vapor Pressure of Dicamba Using the Thermal Evolution Analyzer, unpublished report (1994) (92)

(15) Sandoz Crop Protection Corporation, Determination of the n-octanol/water partition coefficient for dicamba, 1987

(16) ToxiGenics, Inc., Decatur, USA. Teratology study in albino rats with Technical Dicamba. 1981 (102)

(17) U.S. Department of Interior, Fish and Wildlife Service. Handbook of Acute Toxicity of Chemicals to Fish and Aquatic Invertebrates. Resource Publication No. 137. Washington, DC: U.S. Government PrintingOffice, 1980. 27, as cited in HSDB record for dicamba.

(18) Velsicol Chemical Corporation, Acute Toxicity Studies in rats and rabbits, 1974 (99)

(19) Velsicol Chemical Corporation, Hydrolysis of 14C-dicamba, 1981

(20) Velsicol Chemical Corporation, The acute toxicity of banvel technical to the sheepshead minnow Cyprinodon variegatus (BASF 77/5078), 1977 (97)

I U C L I D

Data Set

Existing Chemical	:	ID: 1982-69-0
CAS No.	:	1982-69-0
Generic name	:	3,6-dichloro-2-methoxybenzoic acid, sodium salt
Tag name	:	dicamba, sodium

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 225 °C
Sublimation	:	
Method	:	other: Estimation
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Remark	:	As a salt of a substance melting about 100 C, this material will have a higher MP and be solid at temperaturec below 100 C.
Result	:	SUMMARY MPBPWIN v1.40 Boiling Point: 525.94 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 193.43 deg C (Gold and Ogle Method) Mean Melt Pt : 271.64 deg C (Joback; Gold,Ogle Methods) Selected MP: 224.71 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 1982-69-0 Sodium salt of dicamba
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

25.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .00001 hPa at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Remark	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	Vapor Pressure Estimations (25 deg C): (Using BP: 525.94 deg C (estimated)) (Using MP: 224.71 deg C (estimated)) VP: 2.44E-013 mm Hg (Antoine Method) VP: 4.36E-011 mm Hg (Modified Grain Method) VP: 1.36E-010 mm Hg (Mackay Method) Selected VP: 4.36E-011 mm Hg (Modified Grain Method)
Source	:	Toxicology and Regulatory Affairs, Freeburg IL Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 1982-69-0 Sodium salt of dicamba
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

25.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : = -.9 at °C
pH value :
Method : other (calculated)
Year : 2001
GLP :
Test substance :

Result : Log Kow(version 1.66 estimate): -0.90

SMILES : c1(CL)ccc(CL)c(OC)c1C(=O)O[Na]
CHEM : Dicamba, Sodium salt
MOL FOR: C8 H5 CL2 O3 Na1
MOL WT : 243.02

TYPE	NUM	LOGKOW FRAGMENT	COEFF	VALUE
Frag	1	-CH3	0.5473	0.5473
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	2	-CL	0.6445	1.2890
Frag	1	-O-	-0.4664	-0.4664
Frag	1	-C(=O)O	-0.7121	-0.7121
Factor	1	C(=O)-O-{Na	-3.5500	-3.5500
Const		Equation Constant		0.2290

Log Kow = -0

Source : Toxicology and Regulatory Affairs, Freeburg IL
Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1982-69-0 Sodium salt of dicamba
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
25.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 150 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year : 2001
GLP :
Test substance :

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05
Result : ------ WSKOW v1.40 Results ----------
Log Kow (estimated) : -0.90
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -0.90

Equation Used to Make Water Sol estimate:

Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -0.205
Water Solubility at 25 deg C (mg/L): 1.515e+005

Source : Toxicology and Regulatory Affairs, Freeburg IL
Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1982-69-0 Sodium salt of dicamba
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
25.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Xenon lamp
Light spectrum	:	> 290 nm
Relative intensity	:	1.32 based on intensity of sunlight
Conc. of substance	:	100.19 mg/l at 25 °C
DIRECT PHOTOLYSIS		
Halflife t1/2	:	50.3 day(s)
Degradation	:	31.3 % after 30 day(s)
Quantum yield	:	

Method : A 1000 mL test solution consisting of 100.19 mg dicamba with a specific activity of 412.2 dpm/ug (total 688 kBq) in aqueous buffer solution pH 7 containing 1% acetonitrile was prepared. The test solution was incubated at 25 +/- 1 deg C under contineous stirring for 30 days. Average incident radiation on the reactor surface was 7.704E2 W/m2 (measured before and after the study).
The reaction solution was aerated and connected to a silica gel trap, an ethylene glycol trap (organic volatiles) and a 10% NaOH trap (supposed to collect CO2) in series. Before initiation of photolysis, a 50 mL sample was taken as dark control sample. 20 mL samples were taken before initiation of photolysis and on day 1, 3, 8, 15, 22 and 30.

The samples were analyzed as follows:
- duplicate 1 mL samples were analyzed by LSC
- 15 mL was extracted twice at pH < 1 with ethyl acetate, both fractions were analyzed by LSC (duplicate 1 mL samples)
- ethyl acetate fraction was dried and concentrated, and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- extracted buffer solution of day 15, 22 and 30 were lyophilized followed by acetonitrile extraction; the extract was concentrated and analyzed by TLC using 4 solvent systems (cochromatographed with reference standards)
- duplicate 1 mL ethylene glycol and 10% NaOH trap samples were analyzed by LSC
- silica gel traps were extracted with with methanol, which was then analyzed by LSC; residual radioactivity in the silica traps was determined by combustion
- identity of radioactivity supposed to be CO2 in 10% NaOH trap samples was confirmed for day 22 and 30 by precipitation as BaCO3 and subsequent evolution as CO2 after addition of HCl

On day 30, the reactor was washed with methanol and with acetone. Volumes were measured and 1 mL duplicatealiquots were analyzed by LSC.

Photodegradation was calculated using the SAS Regression Program.A 1000 mL test solution consisting of 100.19 mg dicamba with

Remark : The test substance for this study was dicamba (acid form) rather than the salt. In solution, at pH 7 it does not matter if the salt or acid form is used to prepare the solution.

Result : time point (days) 14C-dicamba (% of actually applied

14C-dicamba)*

0	100 (92.14% of applied 14C)
1	98.83
3	95.25
8	86.87
15	75.62
22	66.44
30	58.74 (degradation: 41.26%)

30 (dark control) 98.61
* calculated by reviewer from % of applied 14C
Unchanged dicamba was confirmed by HPLC.

All other compounds in the different fractions, separated by TLC, were <10% of applied 14C and did not match with reference standards. CO2 in the 10% NaOH trap was 11.7% of applied at day 22 and 16.6% of applied 14C at day 30. Radioactivity in the other traps was <10% of applied 14C at all time points. Reactor wash yielded 0.3% of applied activity. The mass balance was >99% and <103.5% at all time points.

Under these conditions, t1/2 of dicamba was 38.1 days; the photolysis rate constant was 0.018 day-1. Based on the spring sunlight intensity at 40 deg latitude at noon (5.83E2 W/m2) the corresponding photodegradation rate for natural sunlight will be 0.0138 day-1; t1/2 will be 50.3 days.

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1918-00-9 (dicamba), purity 99.6% by l
Conclusion : The photodegradation rate constant in spring sunlight at 40 deg latitude at noon is 0.0138 day-1; t1/2 is 50.3 days. The major photodegradation product is CO2.
Reliability : (2) valid with restrictions
1. In the calculation of t1/2, no correction for the degradation in the dark control was made. However, this will only slightly influence the results, as there was hardly any degradation in the dark control.
2. Except for sterilization of the buffer solution, no measures to guarantee sterility of the samples were described. However, as there was hardly any degradation in the dark control (which was a subsample of the sample to be irradiated), it can be assumed biodegradation was negligible.
Flag : Critical study for SIDS endpoint
25.12.2001 (3)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Degradation : = 0 - 7.6 % after 30 day(s) at pH and °C
Deg. product :
Method : other: essentially OECD 111
Year : 1981
GLP :
Test substance :

Method : Solutions of 10 ppm and 100 ppm dicamba (1.17% and 0.12%

14C-dicamba, respectively) in distilled water or aqueous buffer solutions of pH 5.0, 7.0 and 9.0 were incubated at 25 and 35 deg C for 30 days (volume 201 mL, in amber bottles in shaking water baths). Acetone concentrations were 0.5%. After 1, 7, 14, 21 and 30 days, a duplicate 1-mL sample was taken for radioassay and a duplicate 15-mL sample was taken for extraction using diethyl ether (at pH < 1). Organic and aqueous layers were first radioassayed and then analyzed using TLC and radioautography detection, followed by quantification using LSC. Samples were cochromatographed with dicamba and three metabolite reference standards.

Remark : The test substance for this study was dicamba (acid form) rather than the salt. In solution, at specific pH levels it does not matter if the salt or acid form is used to prepare the solution.

Result : There was no significant dicamba hydrolysis (i.e. equal to or less than 7.6%) at each pH value, both concentrations and both temperatures, except for 100 ppm, pH 7.0, 35 deg C at t=14, 21 and 30 days in the 100 ppm, when degradation was up to 18.5%. Total recovery was only 82.5-83.4% for these samples, whereas it was > 95 for all other samples. Radioactivity remaining in the aqueous phase after extraction was equal to or less than 1% of applied. Three unknown degradation products each constituted less than 4% of applied.

Source : Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 1918-00-9 (14C-dicamba), purity not specified

Conclusion : Dicamba is stable with slight or no hydrolysis over 30 days under the conditions tested.

Reliability : (2) valid with restrictions
1. The fact that at 100 ppm, pH 7.0, 35 deg C up to 18.5% degradation occurred was disregarded because recoveries were low. However, no explanation was given for the low recoveries. It cannot be excluded that loss of radioactivity is due to hydrolysis.
2. Section "Results and discussion" contained 2 values that were not in agreement with values in tables of results.
3. No measures to guarantee sterility of the samples or to exclude oxygen from the solutions were described. However, as measured degradation percentages were very low (except at 100 ppm, pH 7.0, 35 deg C), no significant biotic degradation or oxidation can have occurred.
2. No duplicate samples at any pH.
3. pH 5.0 was tested, whereas OECD 111 prescribes pH 4.

Flag : Critical study for SIDS endpoint

25.12.2001 (6)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media :

Air :

Water :

Soil :

Biota :

Soil :

Method :

Year : 2001

Remark : The Fugacity was determined using the EQC Level III model as

found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the current best estimate for dicamba (from HSDB). Half life in air was determined from the APOWIN program for dicamba (acid) as this would be the likely volatile species. Direct photolysis was not considered in this model. Emissions were restricted to water and soil as it is not volatile. Other parameters used the default values found in EPIWIN.

Result : Full EPIWIN Output:

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : dicamba sodium salt
  Molecular Wt: 221.04
  Henry's LC  : 2.68e-008 atm-m3/mole (Henrywin program)
  Vapor Press : 5.66e-005 mm Hg  (Mpbpwin program)
  Liquid VP   : 0.000413 mm Hg  (super-cooled)
  Melting Pt  : 112 deg C (Mpbpwin program)
  Log Kow     : 2.14  (Kowwin program)
  Soil Koc    : 56.6  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.00528         43           0
   Water     41.4            500          1000
   Soil      58.4            500          1000
   Sediment  0.156           2e+003       0

           Fugacity    Reaction    Advection   Reaction    Advection
            (atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
 Air       6.47e-014    0.945       0.586       0.0472      0.0293
 Water     2.79e-013    638         460         31.9        23
 Soil      2.64e-012    900         0           45          0
 Sediment  2.23e-013    0.601       0.0347      0.0301      0.00174

   Persistence Time: 556 hr
   Reaction Time:    722 hr
   Advection Time:   2.41e+003 hr
   Percent Reacted:  77
   Percent Advected: 23

   Half-Lives (hr), (based upon user-entry):
      Air:      43
      Water:    500
      Soil:     500
      Sediment: 2000

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1982-69-0 Sodium salt of dicamba
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :

Remark : Dicamba has a half life of 31 days with a first-order rate constant of 0.0224/day in a typical midwestern agricultural soil under aerobic conditions. Dicamba is completely mineralized to CO2 under aerobic conditions with 3,6-dichlorosalicylic acid as the only major metabolite. Low levels of 2,3-dihydroxy-3,6-dichlorosalicylic acid were detected. Metabolism under anaerobic conditions is similar to that which occurred in aerobic soil except the rate of dicamba metabolism is reduced under anaerobic conditions.

[Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

AQUATIC FATE: Based on the results of various studies, microbial degradation appears to be the important dicamba removal process in natural water. Photolysis may contribute to dicamba removal from water(Scifres CJ et al; J Environ Qual 2: 306 (1973) As cited in HSDB update of 8-09-2001.

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 1982-69-0 Sodium salt of dicamba
Conclusion : Dicamba (and its soluble salts) biodegrades under both aerobic and anaerobic conditions, it is not know if it can be considered readily biodegradable by the OECD criteria.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 1000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	10
Vehicle	:	water
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: Charles River Breeding Laboraties, Kingston, New York - Age: young adult - Number: 5/sex/dose - Weight at study initiation: 188-269 g - Controls: no ADMINISTRATION: - Doses: 5000 mg/kg bw - Doses per time period: single - Volume administered or concentration: 50% (w/v distilled water); dose volume 10 ml/kg - Post dose observation period: 14 days - food withheld 24 hour pre-dosing till 1 hour after dosing EXAMINATIONS: gross signs of systemic toxicity and mortality (at least twice daily for 14 days). Gross necropsy on visceral and thoracic cavities. BODY WEIGHT: pre-dosing, days 0, 7 and 13 STATISTICAL METHOD: Litchfield and Wilcoxon
Result	:	MORTALITY: - Number of deaths at each dose: no deaths CLINICAL SIGNS: on the day of dosing: lethargy, ataxia, inactivity, salivation, limbs extended and bodies became rigid at touch or sound stimulus and slowed respiration, loose faeces and urine stains. On day 2 after dosing, all animals appeared normal. NECROPSY FINDINGS: no significant gross pathologic findings SEX-SPECIFIC DIFFERENCES: on day 1, all males appeared mildly lethargic, ataxic and inactive while females only appeared slightly affected.
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, 1982-69-0 (sodium salt of Dicamba), puity 20%, impurities not indicated
Conclusion	:	LD50 > 5000 mg/kg bw (= > 1000 mg a.i./kg bw)
Reliability	:	(1) valid without restriction 1. The study was conducted in compliance with GLP. However,

no compliance statement was present.

09.04.2001 (5)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 400 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	10
Vehicle	:	physiol. saline
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: Kings Wheel Rabbitry, Mt. Vernon, Ohio - Age: young adult - Number: 5/sex/dose - Weight at study initiation: 1.65-3.05 kg - Controls: no ADMINISTRATION: - Area covered: 10% of body surface area - Occlusion: yes - Vehicle: slightly moistened with physiological saline - Doses: 2000 mg/kg bw - Removal of test substance: wiped with physiological saline EXAMINATIONS: signs of systemic toxicity and mortality (at least twice daily for 14 days). Gross necropsy on visceral and thoracic cavities. BODY WEIGHT: pre-dosing, days 0, 6 and 13 STATISTICAL METHOD: Litchfield and Wilcoxon
Result	:	MORTALITY: - Number of deaths at each dose: no deaths CLINICAL SIGNS: Moderate to slight erythema and edema (10/10), a brown cast (10/10), slight scaling (10/10), and slight atonia (1/10). BODY WEIGHTS: changes appeared normal. NECROPSY FINDINGS: no significant findings SEX-SPECIFIC DIFFERENCES: no data
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	I, CAS 1982-69-0 (sodium salt of Dicamba), pellets, purity 20%, impurities not indicated
Conclusion	:	LD50 > 2000 mg/kg bw (= > 400 mg a.i./kg bw)

Reliability : (2) valid with restrictions
1. The skin was abraded, which can influence the permeability of the test substance.
2. The study was conducted in compliance with GLP. However no compliance statement was included.

09.04.2001 (4)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

(3) Sandoz Agro, Dicamba: Photodegradation Study in pH 7 Aqueous Solution (1993) (95) unpublished study

(4) Velsicol Chemical Corporation, Acute Dermal Toxicity Study in Albino Rabbits with 20% sodium salt of Dicamba, 1982 (58)

(5) Velsicol Chemical Corporation, Acute Oral Toxicity Study in Albino Rats with 20% sodium salt of Dicamba, 1982 (57)

(6) Velsicol Chemical Corporation, Hydrolysis of 14C-dicamba, 1981

I U C L I D

Data Set

Existing Chemical	:	ID: 68938-79-4
Memo	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium potassium salt
CAS No.	:	68938-79-4
Generic name	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium potassium salt

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 220 °C
Sublimation	:	
Method	:	other: calculated
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== SMILES : c1(CL)ccc(CL)c(OK)c1C(=O)O[Na] CHEM : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt MOL FOR: C7 H2 CL2 O3 Na1 K1 MOL WT : 267.09 --- SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 515.41 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 187.28 deg C (Gold and Ogle Method) Mean Melt Pt : 268.56 deg C (Joback; Gold,Ogle Methods) Selected MP: 219.80 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .000001 at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== SMILES : c1(CL)ccc(CL)c(OK)c1C(=O)O[Na] CHEM : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt MOL FOR: C7 H2 CL2 O3 Na1 K1 MOL WT : 267.09

Vapor Pressure Estimations (25 deg C):
(Using BP: 515.41 deg C (estimated))
(Using MP: 219.80 deg C (estimated))
VP: 7.85E-013 mm Hg (Antoine Method)
VP: 9.27E-011 mm Hg (Modified Grain Method)
VP: 2.81E-010 mm Hg (Mackay Method)
Selected VP: 9.27E-011 mm Hg (Modified Grain Method)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt
CAS 68938-79-4
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. -4.15 at 25 °C
pH value :
Method : other (calculated)
Year : 2001
GLP : no
Test substance :

Method : Estimation using KOWWIN v1.66 in EPIWIN 3.05
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt
CAS 68938-79-4
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 1000 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated from Ko/w estimate
Year : 2001
GLP : no
Test substance :

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05
Result : SMILES : c1(CL)ccc(CL)c(OK)c1C(=O)O[Na]
CHEM : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt
MOL FOR: C7 H2 CL2 O3 Na1 K1
MOL WT : 267.09
----- WSKOW v1.40 Results ----------
Log Kow (estimated) : -4.15
Log Kow (experimental): not available from database

Log Kow used by Water solubility estimates: -4.15

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : 2.393
Log Water Solubility (in moles/L) : 0.573 (Applied Upper Limit)

Water Solubility at 25 deg C (mg/L): 1e+006

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000
Rate constant	:	cm^3/(molecule*sec)
Degradation	:	% after
Method	:	Estimation using APOWIN v1.90 in EPIWIN 3.05
Result	:	AOP Program (v1.90) Results: ========== SMILES : c1(CL)ccc(CL)c(O)c1C(=O)O CHEM : 3,6-Dichloro-2-hydroxybenzoic acid MOL FOR: C7 H4 CL2 O3 MOL WT : 207.01 --- SUMMARY (AOP v1.90): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.6600 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 2.5345 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 3.1945 E-12 cm3/molecule-sec HALF-LIFE = 3.348 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 40.178 Hrs
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid CAS 3401-80-7. This is the form that is expected to be present in air as a vapor.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other: estimated
Year	:	2001
GLP	:	
Test substance	:	
Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis.
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.

The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (3)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type :
Media :
Air :
Water :
Soil :
Biota :
Soil :
Method :
Year : 2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the current best estimate for dicamba (from HSDB). Half life in air was determined from the APOWIN program for the unionized species as this would be the likely volatile species. Direct photolysis was not considered in this model. Emissions were restricted to water and soil as it is not volatile. Other parameters used the default values found in EPIWIN.

Result : Full EPIWIN Output:

```
Level III Fugacity Model (Full-Output):
=======================================
Chem Name: 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt
  Molecular Wt: 267.09
  Henry's LC  : 3.26e-017 atm-m3/mole (calc VP/Wsol)
  Vapor Press : 33.6 mm Hg  (Mpbpwin program)
  Liquid VP   : 2.84e+003 mm Hg  (super-cooled)
  Melting Pt  : 220 deg C (Mpbpwin program)
  Log Kow     : -4.15  (Kowwin program)
  Soil Koc    : 2.9e-005  (calc by model)

           Concentration   Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       6.52e-020       40           0
   Water     56.1            500          1000
   Soil      43.8            500          1000
   Sediment  0.0978          2e+003       0

          Fugacity    Reaction    Advection   Reaction    Advection
           (atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
Air       6.13e-031    1.16e-017   6.7e-018    5.81e-019   3.35e-019
Water     3.51e-022    799         576         39.9        28.8
Soil      1.02e-020    625         0           31.2        0
Sediment  3.07e-022    0.348       0.0201      0.0174      0.00101

   Persistence Time: 514 hr
   Reaction Time:    722 hr
   Advection Time:   1.78e+003 hr
   Percent Reacted:  71.2
   Percent Advected: 28.8

   Half-Lives (hr), (based upon user-entry):
      Air:      40
      Water:    500
      Soil:     500
      Sediment: 2000

   Advection Times (hr):
      Air:      100
      Water:    1000
```

Sediment: 5e+004

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, sodium, potassium salt CAS 68938-79-4
Conclusion : Dicamba (and its soluble salts) biodegrades under both aerobic and anaerobic conditions.
3,6-Dichloro-2-hydroxybenzoic acid has been identified as an intermediate degradation product; therefore, its soluble salts will also biodegrade. It is not known if it can be considered readily biodegradable by the OECD criteria.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	ca. 1562 mg/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1981
GLP	:	no data
Test substance	:	
Remark	:	This value comes from the literature for 2-hydroxy-3,6-dichlorobenzoic acid which is expected to have similar acute toxicity as its soluble salts.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid CAS 3401-80-7.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (4)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

(3) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(4) Pis'ko, GT, Tolstopjatova, GV, and AI Tovstenko AI Comparative study of the toxicity of 2-hydroxy-3,6-dichlorobenzoic acid by various routes of administration Gigiena truda i professional'nye zabolevanija Sep. 1981, No.9, p.55-56.

I U C L I D

Data Set

Existing Chemical	:	ID: 68938-80-7
CAS No.	:	68938-80-7
Generic name	:	3,6-dichloro-2-hydroxybenzoic acid, dipotassium salt

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 220 °C
Sublimation	:	
Method	:	other: estimated
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== SMILES : c1(CL)ccc(CL)c(OK)c1C(=O)OK CHEM : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt MOL FOR: C7 H2 CL2 O3 K2 MOL WT : 283.19 ---------- SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 515.41 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 187.28 deg C (Gold and Ogle Method) Mean Melt Pt : 268.56 deg C (Joback; Gold,Ogle Methods) Selected MP: 219.80 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

25.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .0001 hPa at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== SMILES : c1(CL)ccc(CL)c(OK)c1C(=O)OK CHEM : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt MOL FOR: C7 H2 CL2 O3 K2 MOL WT : 283.19 ------- SUMMARY MPBPWIN v1.40 ----------

Boiling Point: 515.41 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 187.28 deg C (Gold and Ogle Method)
Mean Melt Pt : 268.56 deg C (Joback; Gold,Ogle Methods)
Selected MP: 219.80 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 515.41 deg C (estimated))
(Using MP: 219.80 deg C (estimated))
VP: 7.85E-013 mm Hg (Antoine Method)
VP: 9.27E-011 mm Hg (Modified Grain Method)
VP: 2.81E-010 mm Hg (Mackay Method)
Selected VP: 9.27E-011 mm Hg (Modified Grain Method)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
25.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. -4.15 at 25 °C
pH value :
Method : other (calculated)
Year : 2001
GLP : no
Test substance :

Method : Estimation using KOWWIN v1.66 in EPIWIN 3.05
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 1000 at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: estimated
Year : 2001
GLP : no
Test substance :

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05
Result : Water Sol from Kow (WSKOW v1.40) Results:
==========

Water Sol: 1e+006 mg/L

SMILES : c1(CL)ccc(CL)c(OK)c1C(=O)OK
CHEM : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt
MOL FOR: C7 H2 CL2 O3 K2
MOL WT : 283.19
---------- WSKOW v1.40 Results

Log Kow (estimated) : -4.15
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: -4.15

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : 2.275
Log Water Solubility (in moles/L) : 0.548 (Applied Upper Limit)
Water Solubility at 25 deg C (mg/L): 1e+006

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
25.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	cm³/(molecule*sec)
Degradation	:	% after
Method	:	Estimation using APOWIN v1.90 in EPIWIN 3.05
Result	:	AOP Program (v1.90) Results: ========== SMILES : c1(CL)ccc(CL)c(O)c1C(=O)O CHEM : 3,6-Dichloro-2-hydroxybenzoic acid MOL FOR: C7 H4 CL2 O3 MOL WT : 207.01 ---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.6600 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 2.5345 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 3.1945 E-12 cm3/molecule-sec HALF-LIFE = 3.348 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 40.178 Hrs
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid. CAS 3401-80-7 This is the form of test material that would be present in air as a vapor.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

25.12.2001 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other: estimated
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater

than one year between pH 4 and pH 9.

The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (3)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air :
Water :
Soil :
Biota :
Soil :
Method :
Year : 2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the current best estimate for dicamba (from HSDB). Half life in air was determined from the APOWIN program for dicamba (acid) as this would be the likely volatile species. Direct photolysis was not considered in this model. Emissions were restricted to water and soil as it is not volatile. Other parameters used the default values found in EPIWIN.

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt
  Molecular Wt: 283.19
  Henry's LC  : 3.45e-017 atm-m3/mole (calc VP/Wsol)
  Vapor Press : 9.27e-011 mm Hg  (Mpbpwin program)
  Liquid VP   : 7.83e-009 mm Hg  (super-cooled)
  Melting Pt  : 220 deg C (Mpbpwin program)
  Log Kow     : -4.15  (Kowwin program)
  Soil Koc    : 2.9e-005  (calc by model)

           Concentration   Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       8.5e-018        43           0
   Water     56.1            500          1000
   Soil      43.8            500          1000
   Sediment  0.0978          2e+003       0

           Fugacity    Reaction    Advection   Reaction    Advection
            (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
Air       6.5e-031     1.41e-015   8.74e-016    7.04e-017   4.37e-017
Water     3.51e-022    799         576          39.9        28.8
Soil      1.02e-020    625         0            31.2        0
Sediment  3.07e-022    0.348       0.0201       0.0174      0.00101

   Persistence Time: 514 hr
   Reaction Time:    722 hr
   Advection Time:   1.78e+003 hr
   Percent Reacted:  71.2
   Percent Advected: 28.8

   Half-Lives (hr), (based upon user-entry):
      Air:      43
      Water:    500
      Soil:     500
      Sediment: 2000

   Advection Times (hr):
      Air:      100
      Water:    1000
```

Sediment: 5e+004

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3,6-Dichloro-2-hydroxybenzoic acid, dipotassium salt CAS 68938-80-7
Conclusion : Dicamba (and its soluble salts) biodegrades under both aerobic and anaerobic conditions.
3,6-Dichloro-2-hydroxybenzoic acid has been identified as an intermediate degradation product; therefore, its soluble salts will also biodegrade. It is not known if it can be considered readily biodegradable by the OECD criteria.
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	ca. 1562 ml/kg bw
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	1981
GLP	:	no data
Test substance	:	
Remark	:	This value comes from the literature for 2-hydroxy-3,6-dichlorobenzoic acid which is expected to have similar acute toxicity as its soluble salts.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3,6-Dichloro-2-hydroxybenzoic acid. CAS 3401-80-7
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (4)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Krueger JP et al; J Agric Food Chem 39: 995-9 (1991)]. As cited in HSDB update of 8-09-2001.

(3) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(4) Pis'ko, GT, Tolstopjatova, GV, and AI Tovstenko AI Comparative study of the toxicity of 2-hydroxy-3,6-dichlorobenzoic acid by various routes of administration Gigiena truda i professional'nye zabolevanija Sep. 1981, No.9, p.55-56.

I U C L I D

Data Set

Existing Chemical	:	ID: 583-78-8
CAS No.	:	583-78-8
Molecular Formula	:	Cl2C6H3OH
Generic name	:	2,5-dichlorophenol

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	59 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions Handbook data
Flag	:	Critical study for SIDS endpoint

26.12.2001 (13)

2.2 BOILING POINT

Value	:	211 °C at
Decomposition	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions Handbook data
Flag	:	Critical study for SIDS endpoint

26.12.2001 (13)

2.4 VAPOUR PRESSURE

Value	:	= .08 hPa at 25 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Supported by EPIWIN calculated value value of 0.06 hPa
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Reliability	:	(2) valid with restrictions Literature value
Flag	:	Critical study for SIDS endpoint

26.12.2001 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 3.06 at 25 °C
pH value	:	

Remark	:	Supported by EPIWIN calculated value value of 2.80
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-dichlorophenol, CAS 583-78-8
Reliability	:	(2) valid with restrictions Literature value
Flag	:	Critical study for SIDS endpoint

26.12.2001 (6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 2000 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	other: slightly soluble
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	

Remark	:	Remarks: 1. Secondary literature. No source or method of determination is given. There is an experimental database match given in WSKOW v1.40 in EPIWIN 3.05 Experimental Water Solubility Database Match: Name : 2,5-DICHLOROPHENOL CAS Num : 000583-78-8 Exp WSol : 2000 mg/L (25 deg C) Exp Ref : CHEM INSPECT TEST INST (1992)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(4) not assignable secondary literature (remark 1)
Flag	:	Critical study for SIDS endpoint

26.12.2001 (3) (5)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	ca. .000000000007 cm³/(molecule*sec)
Degradation	:	= 50 % after 18 hour(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	

Method : Estimation using APOWIN v1.90 in EPIWIN 3.05

Result :

AOP Program (v1.90) Results:
==========
SMILES : c1(CL)ccc(CL)c(O)c1
CHEM : 2,5-Dichlorophenol
MOL FOR: C6 H4 CL2 O1
MOL WT : 163.00
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS

Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 6.8451 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 6.9851 E-12 cm3/molecule-sec
HALF-LIFE = 1.531 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 18.375 Hr

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-dichlorophenol, CAS 583-78-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (5)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	
Test substance	:	

Method : Estimated on chemical principles based on absence of groups susceptible to hydrolysis

Remark	:	The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-dichlorophenol, CAS 583-78-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (14)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	
Water	:	
Soil	:	
Biota	:	
Soil	:	
Method	:	
Year	:	2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Measured values were used for physical constants. Biodegradation was based on the current best estimate (from HSDB). Half life in air was determined from the APOWIN program. Direct photolysis was not considered in this model. Other parameters used the default values found in EPIWIN

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 2,5-Dichlorophenol
  Molecular Wt: 163
  Henry's LC  : 4.77e-007 atm-m3/mole (Henrywin program)
  Vapor Press : 0.06 mm Hg  (user-entered)
  Liquid VP   : 0.13 mm Hg  (super-cooled)
  Melting Pt  : 59 deg C (user-entered)
  Log Kow     : 3.06  (user-entered)
  Soil Koc    : 471  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       4.47           24          1000
   Water     31.5           125         1000
   Soil      63.9           200         1000
   Sediment  0.136          400         0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
Air       3.34e-011    644         223         21.5        7.43
Water     2.3e-012     870         157         29          5.23
Soil      4.47e-012    1.1e+003    0           36.8        0
Sediment  4.03e-013    1.17        0.0136      0.0392      0.000452

   Persistence Time: 166 hr
   Reaction Time:    190 hr
   Advection Time:   1.31e+003 hr
   Percent Reacted:  87.3
   Percent Advected: 12.7


   Half-Lives (hr), (based upon user-entry):
      Air:      24
      Water:    125
      Soil:     200
      Sediment: 400
```

```
Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 2,5-dichlorophenol, CAS 583-78-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (5)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Contact time : 4 day(s)
Degradation : = 52 (±) % after 4 day(s)
Result :
Deg. product :
Method :
Year : 1966
GLP : no data
Test substance :

Remark : The material is reported to undergo 54% ring degradation in 4 days with acclimated sludge, it cannot be setermined if this test substance is considered readily biodegradable by OECD criteria.
Result : The biological degradation of chlorophenols in activated sludge /was studied/. 2,5-Dichlorophenol was more resistent to degradation than 2,4-dichlorophenol. While 2,4-dichlorophenol was 100% degraded, including ring degradation, in five days, 2,5-dichlorophenol was only 52% ring-degraded in four days.

[USEPA; Ambient Water Quality Criteria Doc: Chlorinated Phenols p.C-29 (1980) EPA 440/5-80-032]**PEER REVIEWED** As cited in HSDB update of 8-09-2001
Source : Toxicology and Regulatory Affairs Flemington NJ
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (8)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2475 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	female
Number of animals	:	10
Vehicle	:	other: sesame oil
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source:no data
- Age: no data
- Number:10/dose
- Weight at study initiation: 80-97 g
- Controls: no

ADMINISTRATION:
- Doses: 1600, 2500, 4000 mg/kg bw
- Doses per time period: single (gavage)
- Volume administered not indicated
- Post dose observation period: 14 days
- food withheld 16 hr before to 2 hr after dosing

EXAMINATIONS: Necropsy of all animals with macroscopic examination. Body weight (pre-dosing, days 7 and 14)

STATISTICAL METHOD: probit (Linder and Weber)

Result :

MORTALITY:
- Number of deaths at each dose: 1600, 2500 and 4000 mg/kg bw
1/10, 4/10 and 10/10
- Time of death: deaths within 24 hours after dosing

CLINICAL SIGNS: in dying animals: excessive breathing, equilibrium disturbance and tremor, moreover tonic clonic spasms in the ventral region. In the highest dose, these signs occurred immediately after dosing.

NECROPSY FINDINGS: No abnormal findings were noted in surviving animals.
In decendents: clear dilated bloodvessels on the intestines

BODY WEIGHT: normal body weight gain in surviving animals
No data on decendents

POTENTIAL TARGET ORGANS: intestines

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-Dichlorphenol), purity not indicated, cristalline form
Conclusion	:	LD50 2475 mg/kg bw (95% CI 2101-2916 mg/kg bw)
Reliability	:	(2) valid with restrictions 1. The information was essentially confined to what is

included in the current summary
2. only females were tested
3. no individual data were present

02.04.2001 (7)

Type	:	LD50
Value	:	946 - 1600 ml/kg bw
Species	:	mouse
Strain	:	other: CD-1 ICR
Sex	:	male/female
Number of animals	:	100
Vehicle	:	other: corn oil
Doses	:	
Method	:	other: not indicated
Year	:	
GLP	:	no data
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Age: adult
- Number: 10 males, 10 females per dosage level
- Weight at study initiation:
- Controls: no data

ADMINISTRATION:
- by gavage
- Doses: 5 levels, levels not indicated
- Volume administered or concentration: 10 mL/kg body weight
- food withheld for 2 h after dosing
- Post dose observation period: 14 days

EXAMINATIONS: behavior and visible health, time of death, necropsy of animals that died during the test

STATISTICAL METHOD: Log probit analysisof Finney; Litchfield, Wilcoxon.

Remark	:	Remarks: 1. Remarks: The article contains a summary rather than a full report. Information is essentially confined to what is mentioned in this summary. Especially no detailed results are given.
Result	:	LD50 male: 1600 mg/kg bw (confidence limits: 1233-2075 mg/kg bw); LD50 female: 946 mg/kg bw (confidence limits: 623-1438 mg/kg bw)
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity 98%
Reliability	:	(4) not assignable secondary literature (remark 1)
Flag	:	Critical study for SIDS endpoint

15.03.2001 (2)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 185000 mg/m³
Species	:	rat
Strain	:	other: Spartan
Sex	:	male/female
Number of animals	:	10

Vehicle	:	
Doses	:	
Exposure time	:	4 hour(s)
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: no data - Age: no data - Weight at study initiation: 216-243 g - Number of animals: 10 (5 male, 5 female) ADMINISTRATION: - Type of exposure: inhalation (whole body) - Exposure duration: 4 hours - Concentrations: 50000 mg/m3; 185000 mg/m3 - Particle size: no data - Type or preparation of particles: no data - Air changes: no data EXAMINATIONS: clinical signs during and immediately following exposure; macroscopy
Result	:	MORTALITY: - Number of deaths at each dose:50000 mg/m3: none; 185000 mg/m3: 2 (females) - Time of death: during exposure (both) CLINICAL SIGNS: 50000 mg/m3, (all rats): increased/decreased motor activity, eye squint, erythema, lacrimation, salivation, clear nasal discharge, ocular and nasal porphyrin discharge, slight dispnoea. The symptoms disappeared in all rats 24 hours after exposure 185000 mg/m3, (all rats): The same symptoms as at 50000 mg/m3, with addition of marked dispnoea, corneal opacity, ataxia, sedation and body jerking. The symptoms disappeared 72 hours after exposure (one rat exhibiting nasal porphyrin discharge at day 10) NECROPSY FINDINGS: congested lungs and liver, slight corneal opacity (in the animals that died)
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions 1. The information included in the report was confined to what is included in the current summary 2. No information on body weight was presented

09.04.2001 (10)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 8000 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	4
Vehicle	:	

Doses	:	
Method	:	
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: no data - Age: no data - Weight at study initiation: 2387-2970 g - Controls: no data ADMINISTRATION: - Area covered: no data - Occlusion: yes - Vehicle: not applicable (applied as powder) - Doses: 1000, 2000, 4000 and 8000 mg/kg bw - Removal of test substance: washed with tepid tap water EXAMINATIONS: observations for mortality during 14 days; body weight at start and day 14 STATISTICAL METHOD: Thompson, W.R., Bact. Rev.: 115-145, 1947
Result	:	MORTALITY: - Number of deaths at each dose: none CLINICAL SIGNS: no data BODY WEIGHT: decreased body weight in both females at 2000 mg/kg bw , in one male and one female at 4000 mg/kg bw and in males at 8000 mg/kg
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified
Reliability	:	(2) valid with restrictions 1. The information included in the report was confined to what is included in the current summary 2. Only 4 animals per group (animals not of one sex only), of which one underwent skin abrasion (OECD 402: at least five animals per dosage group, no abrading of the skin) 3. The size of the application area was not indicated

09.04.2001 (11)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	4 weeks
Frequency of treatm.	:	5 days/week, 6 hours/day
Post exposure period	:	
Doses	:	0.1, 0.3 and 1.0 mg/L
Control group	:	yes, concurrent no treatment

LOAEL	:	= .1 mg/l
Method	:	other: not indicated
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS
- Age: 8 weeks
- Weight at study initiation: males 206-230 g,females 192-224 g
- Number of animals: 10/sex/treatment

ADMINISTRATION / EXPOSURE
- Exposure period: 4 weeks, 6 hours/day, 5 days/week
- Route of administration: inhalation (whole body)
- Doses: 0.1, 0.3 and 1.0 mg/L
- Particle size: not applicable (vapour)
- Air changes: 2-16/hour

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality/clinical signs: twice daily
- Body weight: pre-treatment and weekly thereafter
- Haematology: after 4 weeks: haematocrit, Hb, erythrocyte count, (differential) leucocyte count, MCV, MCH(C).
- Biochemistry: after 4 weeks: glucose, BUN, ALP, ALAT, ASAT
- Urinalysis: after 4 weeks accoridng to OECD 407

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: liver, spleen, kidneys, heart, lungs, brain, adrenals, thyroid, pituitary
- Macroscopic: all tissues (see microscopy) from all animals
- Microscopic: from controls and high dose group: nasal turbinates, trachea, lung, spleen, pancreas, stomach, duodenum, uterus, prostate, kidneys, urinary bladder, ovaries, testes, bone marrow, heart, mediastinal and mesenteric lymphnodes, colon, liver, adrenals, olfactory bulb, thyroid, parathyroid, brain , eye, pituitary, gross lesions
from other dose groups: nasal turbinates, trachea, lung, liver

ANALYSES:
- Method: nominal concentrations by weighing of the vaporisation flask before and after exposure

STATISTICAL METHODS: ANOVA, Bartlett's test, Dunnett's test

Result :

ANALYSES:
- Nominal concentration: at 0.1, 0.3 and 1.0 mg/L 0.07-0.28, 0.07-1.09 and 0.45-1.36 mg/L respectively.

TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality: none
- Clinical signs:
Nasal irritation with or without discharge in all treatment groups and controls
Ocular irritation and discharge in all treatment groups
Salivation in 8 males and 4 females at 0.3 mg/L and in 7 males and 7 females at 1.0 mg/L
Dyspnoea in one male and 7 females at 0.3 mg/L
Incidental findings respiratory distress, skin irritation, cloudy spots on eyes, decreased activity and soaked abdomen

- Body weight gain: decreased at 0.3 mg/L during week 2-4 and at 1.0 during week 1-4.
- Haematology:
Hb increased at the high dose group,
No. of leucocytes increased in females at 0.3 and 1.0 mg/L
- Clinical chemistry:
ASAT increased in high dose males and females
- Urinalysis: no treatment related effects
- Organ weights:
Decreased absolute liver and brain weight in males at 0.3 and 1.0 mg/L
Increased relative lung weight in females at 1.0 mg/L
Decreased absolute heart weight in males at 0.3 mg/L
Increased relative kidney weight in all treated males
- Gross pathology:
Brown cyanotic/discolored areas, foci and atelectasis in the lungs were seen in 1-2 animals/sex/treatment and in controls. At 1.0 mg/L the incidence was slightly increased in females.
Other incidental effects included haemorrhagic/hyperemic lymphnodes, effects on stomach mucosa, pale/discolored liver areas/foci and haemorrhagic foci and discoloration of the kidneys.
- Histopathology:
Inflammatory cell and lymphocyte infiltrate, macrophage aggregation and septal fibrosis in the lungs of all treated animals
Inflammation of the nasal cavity (mucosa) in animals at 1.0 mg/L
Lymphocytic infiltrate, inflammation, foci and necrosis of the liver in treated and control animals. The incidence in control animals was slightly lower (9/20) compared to treatd animals (14-16/20).

STATISTICAL RESULTS: The effects on body weight, organ weight and bloodparameters were statistically significant. None of the effects showed a clear concentration-response relationship.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified

Conclusion : LOAEL 0.1 mg/L based on liver effects.
Other effects seen were related to a weight decrease (organ weights) or could be attributed to irritant properties of the test substance (effects in the respiratory tract).

Reliability : (2) valid with restrictions
1 No analyses for actual concentration, homogeneity and stability were performed.
2 The effects on organ weights are expected to be related to the decreased body weight.
3 No blood clotting parameters were detemined

09.04.2001 (12)

Type :
Species : rabbit
Sex : male/female
Strain : New Zealand white
Route of admin. : dermal
Exposure period : 21 days
Frequency of treatm. : 5 days/week, 6 hours/day
Post exposure period :
Doses : 1.0, 10 and 100 mg/kg bw

Control group : other: distilled water
Method : other: not indicated
Year :
GLP : no
Test substance : other TS

Method : TEST ORGANISMS
- Weight at study initiation: 2171-2921 g (males), 2028-3146 g (females)
- Number of animals: 4/sex/treatment
- Source: HARE Rabbits Research, Hewitt, NJ

ADMINISTRATION / EXPOSURE
- Exposure period: 21 days, 5 days/week, 6 hours/day
- Route of administration: dermal
- Doses: 1.0, 10.0 and 100 mg/kg bw; water control
- Vehicle: not applicable (substance was melted at 60 C before application)
- Total volume applied: =<0.1 mL/kg
- Area treated: 10% of body surface (at 1.0 and 10 mg/kg bw every day another area was treated)
- Occlusion: no (a collar was applied to prevent oral ingestion of the test substance)
- Removal of test substance: washed with tepid water after 6 hours

CLINICAL OBSERVATIONS AND FREQUENCY:
- Mortality/clinical signs: daily
- Dermal effects: before and after exposure
- Body weight: weekly
- Haematology/biochemistry: pre-test and after 21 days: haematocrit, Hb, erythrocyte count, (differential) leucocyte count, MCV, MCH(C)
glucose, BUN, ALP, ALAT, ASAT
- Urinalysis: pre-test and after 21 days according to OECD 410

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: liver, spleen, kidneys, brain, adrenals, thyroid, testes, ovaries
- Macroscopic: all tissues (see microscopy) from all animals
- Microscopic: from all animals: skin, brain, lung, spleen, pancreas, stomach, small and large intestines, kidneys, urinary bladder, gallbladder, ovaries, testes, bone marrow, heart, prefemorral and mesenteric lymphnodes, liver, adrenals, thyroid, parathyroid, eye, pituitary, sciatic nerve, spinal cord, thymus, skeletal muscle, gross lesions

STATISTICAL METHODS: ANOVA, Bartlett's test, t-test (Steel), Dunnett's test

Result : TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
- Mortality and time to death: one male at 10 mg/kg bw on day 20 and 3 females at 100 mg/ kg bw during week 3
- Clinical signs: In males at 100 mg/kg bw red swollen eye, ocular and/or nasal discharge were seen.
In animals that died diarrhoea was apparent on the day before death
- Dermal effects:
Skin effects were seen at all dose groups with increasing incidence and severity. At 1.0 mg/kg bw effects were

restricted to erythema and oedema in all animals. At 10 mg/kg bw atonia and corisceousness were seen next to erythema and oedema. At 100 mg/kg bw fissuring of the skin and desquamation was seen in addition to erythema, oedema, atonia and corisceousness
- Body weight gain: no treatment related effects
- Haematology:
At 10 and 100 mg/kg bw the number of erythrocytes was increased in males. At 100 mg/kg bw an increased haemoglobin level was reported in males. Leucocyte counts were increased in males and females at 10 mg/kg bw and in males at 100 mg/kg bw
- Clinical chemistry:
BUN and ALAT were decreased in the surviving female at 100 mg/kg bw
- Urinalysis:
A decreased volume was reported in males at 1.0 and 100 mg/kg bw; specific gravity was increased at 1.0 mg/kg bw
- Organ weights:
Liver weight was decreased in females at 1.0 and 10 mg/ kg bw (both absolute and relative)
Relative spleen weight was decreased in mid and high dosed females
Absolute kidney weight and absolute and relative adrenal weight were decreased in females at 10 mg/kg bw
- Gross pathology:
Skin lesionss at the application site consisting of thickening, encrustation, sloughing, necrosis, leatherness, foci in the dermis and epidermis were reported in all treated animals
- Histopathology:
Skin effects (application site) included inflammatory cell infiltrate, acanthosis, hyperkeratosis and necrotic exudate on the epidermal surface at 1.0 mg/kg bw. At 10 and/or 100 mg/kg bw additionally dermal fibroplasia and ulceration was reported.
At 100 mg/kg hyperplasia of the lymphnodes was seen.
Other incidental findings included areas of asperm and ectatic tubuli in the testes, lung congestion, lymphoid infiltrate in the liver, meningitis, nodules in the brain, cysts in the thyroid.
Several animals showed an infection of coccidia in their small intestine

STATISTICAL RESULTS: Effects on RBC and HB and liver weight reached a level of statistical significance

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : II, CAS 583-78-8 (2,5-dichlorophenol), purity not specified

Conclusion : Based on local effects the LOAEL is 1.0 mg/kg bw.
For systemic effects a NOAEL of 100 mg/kg bw can be derived.
The lymphnode hyperplasia was considered secondary to skin effects.

Reliability : (2) valid with restrictions
1 No analyses were performed to check the actual amount of test substance applied.
2 The number of animals/treatment was too small. Abrasion of the skin of half of the animals did not seem to influence the results, but is not requested by the OECD guideline
3 Effects on blood parameters remained within historical values.
4 The liver effects were only seen in females and showed no

relationship with dose or microscopic changes. Therefore they were considerd to be not related to treatment.

09.04.2001 (9)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	HGPRT assay
System of testing	:	CHO-cells (K1-BH4)
Test concentration	:	62.5-250 ug/mL
Cycotoxic concentr.	:	200 ug/mL
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: not indicated
Year	:	
GLP	:	no data
Test substance	:	other TS

Method :

SYSTEM OF TESTING
- Species/cell type: CHO-K1-BH4
- Proficiences: HGPRT
- Metabolic activation system: Arochlor-1254-induced male rat liver homogenate

ADMINISTRATION:
- Dosing: with and without S9 100, 125, 150, 200 and 250 ug/mL; additionally with S9 62.5 and 75 ug/mL
- Number of replicates: one
- Positive and negative control: 5-Bromo 2'deoxyuridine (-S9), 3-methylcholanthrene (+S9) and DMSO (vehicle)
Exposure time: 1.5E06 cells were exposed for 4 h followed by 6-7 day expression time

CRITERIA FOR EVALUATING RESULTS:
- Statistical method: Kastenbaum and Baumann

Result : GENOTOXIC EFFECTS:
- With metabolic activation: negative
- Without metabolic activation: negative

FREQUENCY OF EFFECTS: number of mutants remained within (negative) control ranges with the exception of the number of mutants in the lowest dose tested with S9-mix. Positive controls gave the expected results

PRECIPITATION CONCENTRATION: not observed

CYTOTOXICITY (% of control survival) at the highest tested concentration:
- With metabolic activation: 0.4% at 250 ug/mL
- Without metabolic activation: 20% at 250 ug/mL

STATISTICAL RESULTS: The increase of the number of mutants at 62.5 ug/mL (+S9) was statistically significant

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : II, CAS 583-78-8 (2,5-dichlorophenol), purity >98%

Reliability : (2) valid with restrictions
1. The report is limited to the above mentioned.
2. The increased number of mutants seen at 62.5 ug/mL in the assay with metabolic activation is considered to be not relevant, since no concentration effect relationship was

observed.

06.04.2001 (1) (15)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	NMRI
Route of admin.	:	gavage
Exposure period	:	single dose
Doses	:	1500 mg/kg bw
Result	:	negative
Method	:	other: not indicated
Year	:	
GLP	:	no data
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Age: 8-12 weeks
- Weight at study initiation: not indicated
- No. of animals: 10/treatment

ADMINISTRATION:
- Vehicle: corn oil
- Frequency of treatment: single dose by oral gavage (volume 5 ml/kg)
- Sampling times: 24, 48 and 72 hours after treatment (samples from 10 animals each time, number of bone marrow smears not indicated)
- Control groups and treatment:
negative: corn oil (5 ml/kg)
positive: cyclophosphamide (20 mg/kg bw in deionised water)

EXAMINATIONS:
- % of polychromatic erythrocytes (PCE) in 1000 erythrocytes
- Number of micronucleated PCE/1000 PCE

CRITERIA FOR EVALUATING RESULTS:
- Statistical method: Wilcoxon's non-parametric rank sum test

Result : TOXIC RESPONSE/EFFECTS BY DOSE LEVEL:
Not reported

EFFECT ON PCE/NCE RATIO:
% PCE 44.6, 32.0 and 27.6 at 24, 48 and 72 hours, resp.

GENOTOXIC EFFECTS:
Mean number of micronucleated PCE: 0.6, 1.4 and 0.9 at 24, 48 and 72 hours sampling time, resp.

STATISTICAL RESULTS:
% PCE significantly decreased at the 72-hours sampling time

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	II, CAS 583-78-8 (2,5-dichlorophenol), purity >98%
Conclusion	:	not clastogenic
Reliability	:	(2) valid with restrictions 1. The report was limited to the above mentioned. 2. The proportion of micronucleated PCE was determined for

1000 PCE. This is in agreement with OECD 474 (1983); OECD 474 (1997) requires evaluation of 2000 PCE.

06.04.2001 (1) (15)

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Bayer, Investigations on the mutagenicity of 1,4-dichlorobenzene and its main metabolite 2,5-dichlorophenol in vivo and in vitro, 2000

(2) Borzelleca J.F., Condie L.W. & Hayes J.R. Toxicological evaluation of selected chlorinated phanols Water chlorination: Chem. Envirn. Impact Health eff. Proc. Conf. 5K (1985) (1)

(3) Borzelleca J.F., Condie L.W. & Hayes J.R. Toxicological evaluation of selected chlorinated phanols Water chlorination: Chem. Envirn. Impact Health eff. Proc. Conf. 5K (1985) (25)

(4) Dolfing J, Harrison BK; Environ Sci Technol 26: 2213-93 (1991), As cited in HSDB update of 8-09-2001

(5) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(6) Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995. 15, As cited in HSDB update of 8-09-2001

(7) Hoechst Aktiengesellschaft, Akute orale Toxizitaet von 2,5-Dichlorphenol an weiblichen SPF-Wistar-Ratten, 1976 (3)

(8) Ingols RS et al; J Water Pollut Control Fed 38: 629-35 (1966) As cited in HSDB update of 8-09-2001

(9) International Research and Development Corporation, 2,5-dichlorophenol: 3-week dermal toxicity study in rabbits, 1980 (1)

(10) International Research and Development Corporation, 2,5-dichlorophenol: acute toxicity studies in rats and rabbits, 1974

(11) International Research and Development Corporation, 2,5-dichlorophenol: acute toxicity studies in rats and rabbits, 1974 (108)

(12) International Research and Development Corporation, 2,5-Dichlorophenol Four-week inhalation study in rats, 1980 (2)

(13) Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 76th ed. Boca Raton, FL: CRC Press Inc., 1995-1996.,p. 3-254

(14) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(15) Tegethoff K., Investigations on the mutagenicity of 1,4-dichlorobenzene and its main metabolite 2,5-dichlorophenol in vivo and in vitro, Mutat Res 470: 161-167, 2000 (22)

I U C L I D

Data Set

Existing Chemical	:	ID: 52166-72-0
CAS No.	:	52166-72-0
Generic name	:	2,5-dichlorophenol, sodium salt

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 202 °C
Sublimation	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	--------- SUMMARY MPBPWIN v1.40 ----------

Boiling Point: 476.56 deg C (Adapted Stein and Brown Method)

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 164.60 deg C (Gold and Ogle Method)
Mean Melt Pt : 257.22 deg C (Joback; Gold,Ogle Methods)
Selected MP: 201.65 deg C (Weighted Value)

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Sodium 2,5-dichlorophenol CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .00001 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	---------- SUMMARY MPBPWIN v1.40 -

Vapor Pressure Estimations (25 deg C):
(Using BP: 476.56 deg C (estimated))
(Using MP: 201.65 deg C (estimated))
VP: 4.71E-011 mm Hg (Antoine Method)
VP: 1.46E-009 mm Hg (Modified Grain Method)
VP: 4.04E-009 mm Hg (Mackay Method)
Selected VP: 1.46E-009 mm Hg (Modified Grain Method)

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Sodium 2,5-dichlorophenol CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	ca. .12 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	

Method	:	Estimation using KOWWIN v1.66 in EPIWIN 3.05
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Sodium 2,5-dichlorophenol CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	ca. 40000 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	2001
GLP	:	no
Test substance	:	

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05

Result :

```
--- WSKOW v1.40 Results ----------------------
Log Kow  (estimated)  :  0.12
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  0.12

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW +
Correction
      (used when Melting Point NOT available)

     Correction(s):        Value
     --------------------  -----
      No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -0.649
   Water Solubility at 25 deg C (mg/L):  4.147e+00
```

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Sodium 2,5-dichlorophenol CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	cm³/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	

Method	:	Estimation using APOWIN v1.90 in EPIWIN 3.05
Remark	:	The indirect photolysis rate was estimated using 2,5-dichlorophenol as that is the species most likely to exist in the vapor state.
Result	:	AOP Program (v1.90) Results: ========== SMILES : c1(CL)ccc(CL)c(O)c1 CHEM : 2,5-Dichlorophenol MOL FOR: C6 H4 CL2 O1 MOL WT : 163.00 ---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 6.8451 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 6.9851 E-12 cm3/molecule-sec HALF-LIFE = 1.531 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 18.375 Hrs
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-Dichlorophenol CAS 583-79-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

3.1.2 STABILITY IN WATER

Type	:	
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	

Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark	:	The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Sodium 2,5-dichlorophenol CAS 52166-72-0
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (3)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	
Year	:	2001

Method :

The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the current best estimate for 2,5-dichlorophenol (from HSDB). Half life in air was determined from the APOWIN program for 2,5-dichlorophenol as this would be the likely volatile species. Direct photolysis was not considered in this model. Emissions were restricted to water and soil as this test substance it is not volatile. Other parameters used the default values found in EPIWIN

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Sodium 2,5-Dichlorophenol
  Molecular Wt: 184.99
  Henry's LC  : 5.49e-007 atm-m3/mole (Henrywin program)
  Vapor Press : 1.46e-009 mm Hg  (Mpbpwin program)
  Liquid VP   : 8.16e-008 mm Hg  (super-cooled)
  Melting Pt  : 202 deg C (Mpbpwin program)
  Log Kow     : 0.12  (Kowwin program)
  Soil Koc    : 0.54  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.131           24           0
   Water     44              125          1000
   Soil      55.8            200          1000
   Sediment  0.0522          400          0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
Air       5.92e-014    15.6        5.4         0.779       0.27
Water     2.68e-012    1e+003      181         50.1        9.04
Soil      1.21e-010    795         0           39.8        0
Sediment  1.57e-012    0.371       0.00429     0.0186      0.000214

   Persistence Time: 206 hr
   Reaction Time:    227 hr
   Advection Time:   2.21e+003 hr
   Percent Reacted:  90.7
   Percent Advected: 9.31
```

```
Half-Lives (hr), (based upon user-entry):
   Air:      24
   Water:    125
   Soil:     200
   Sediment: 400

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Sodium 2,5-dichlorophenol CAS 52166-72-0
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Contact time : 4 day(s)
Degradation : = 54 (±) % after 4 day(s)
Result :

Remark : The free phenol form of this material is reported to undergo 54% ring degradation in 4 days with acclimated sludge, it cannot be determined if this test substance is considered readily biodegradable by OECD criteria
Result : The biological degradation of chlorophenols in activated sludge was studied. 2,5-Dichlorophenol was more resistent to degradation than 2,4-dichlorophenol. While 2,4-dichlorophenol was 100% degraded, including ring degradation, in five days, 2,5-dichlorophenol was only 52% ring-degraded in four days. [USEPA; Ambient Water Quality Criteria Doc: Chlorinated Phenols p.C-29 (1980) EPA 440/5-80-032]**PEER REVIEWED** As cited in HSDB record for 2,5-dichlorophenol, update of 8-09-2001
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 2,5-Dichlorophenol CAS 583-79-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Ingols RS et al; J Water Pollut Control Fed 38: 629-35 (1966) As cited in HSDB update of 8-09-2001

(3) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

I U C L I D

Data Set

Existing Chemical	:	ID: 68938-81-8
CAS No.	:	68938-81-8
Generic name	:	2,5-dichlorophenol, potassium salt

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 201 °C
Sublimation	:	
Method	:	other: Calculated
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)ccc(CL)c(OK)c1 CHEM : Potassium 2,5-Dichlorophenol MOL FOR: C6 H3 CL2 O1 K1 MOL WT : 201.09 ---- SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 476.56 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 164.60 deg C (Gold and Ogle Method) Mean Melt Pt : 257.22 deg C (Joback; Gold,Ogle Methods) Selected MP: 201.65 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Potassium 2,5-dichlorophenol CAS 68938-81-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .00001 hPa at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)ccc(CL)c(OK)c1 CHEM : Potassium 2,5-Dichlorophenol MOL FOR: C6 H3 CL2 O1 K1 MOL WT : 201.09

-- SUMMARY MPBPWIN v1.40 ----------

Vapor Pressure Estimations (25 deg C):
(Using BP: 476.56 deg C (estimated))
(Using MP: 201.65 deg C (estimated))
VP: 4.71E-011 mm Hg (Antoine Method)
VP: 1.46E-009 mm Hg (Modified Grain Method)
VP: 4.04E-009 mm Hg (Mackay Method)
Selected VP: 1.46E-009 mm Hg (Modified Grain Method

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium 2,5-dichlorophenol CAS 68938-81-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. .12 at °C
pH value :
Method : other (calculated)
Year : 2001
GLP : no
Test substance :

Method : Estimation using KOWWIN v1.66 in EPIWIN 3.05
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium 2,5-dichlorophenol CAS 68938-81-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 34 g/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05
Result :

Water Sol from Kow (WSKOW v1.40) Results:
==========

Water Sol: 3.441e+004 mg/L

SMILES : c1(CL)ccc(CL)c(OK)c1
CHEM : Potassium 2,5-Dichlorophenol
MOL FOR: C6 H3 CL2 O1 K1
MOL WT : 201.09

---------- WSKOW v1.40 Results

Log Kow (estimated) : 0.12
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 0.12

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -0.767
Water Solubility at 25 deg C (mg/L): 3.441e+00

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium 2,5-dichlorophenol CAS 68938-81-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	cm³/(molecule*sec)
Degradation	:	% after
Method	:	Estimation using APOWIN v1.90 in EPIWIN 3.05
Remark	:	The indirect photolysis rate was estimated using 2,5-dichlorophenol as that is the species most likely to exist in the vapor state.
Result	:	AOP Program (v1.90) Results: ========== SMILES : c1(CL)ccc(CL)c(O)c1 CHEM : 2,5-Dichlorophenol MOL FOR: C6 H4 CL2 O1 MOL WT : 163.00 SUMMARY (AOP v1.90): HYDROXYL RADICALS ---------- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Aromatic Rings = 6.8451 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 6.9851 E-12 cm3/molecule-sec HALF-LIFE = 1.531 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 18.375 Hrs
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-Dichlorophenol CAS 583-79-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark	:	The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.

Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Potassium 2,5-dichlorophenol CAS 68938-81-8
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (3)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	
Water	:	
Soil	:	
Biota	:	
Soil	:	
Method	:	
Year	:	2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the current best estimate for 2,5-dichlorophenol (from HSDB). Half life in air was determined from the APOWIN program for 2,5-dichlorophenol as this would be the likely volatile species. Direct photolysis was not considered in this model. Emissions were restricted to water and soil as this test substance it is not volatile. Other parameters used the default values found in EPIWIN.

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Potassium 2,5-Dichlorophenol
  Molecular Wt: 201.09
  Henry's LC  : 1.12e-014 atm-m3/mole (calc VP/Wsol)
  Vapor Press : 1.46e-009 mm Hg  (Mpbpwin program)
  Liquid VP   : 8.16e-008 mm Hg  (super-cooled)
  Melting Pt  : 202 deg C (Mpbpwin program)
  Log Kow     : 0.12  (Kowwin program)
  Soil Koc    : 0.54  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.15e-013       24           0
   Water     43.6            125          1000
   Soil      56.4            200          1000
   Sediment  0.0517          400          0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
Air       4.82e-026    1.38e-011   4.77e-012   6.89e-013   2.39e-013
Water     5.06e-020    1.01e+003   181         50.3        9.07
Soil      2.32e-018    813         0           40.6        0
Sediment  2.96e-020    0.373       0.0043      0.0186      0.000215

   Persistence Time: 208 hr
   Reaction Time:    229 hr
   Advection Time:   2.29e+003 hr
   Percent Reacted:  90.9
   Percent Advected: 9.07

   Half-Lives (hr), (based upon user-entry):
      Air:      24
      Water:    125
      Soil:     200
      Sediment: 400

   Advection Times (hr):
      Air:      100
```

```
Water:    1000
Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium 2,5-dichlorophenol CAS 68938-81-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Contact time : 4 day(s)
Degradation : = 54 (±) % after 4 day(s)
Result :

Remark : The free phenol form of this material is reported to undergo 54% ring degradation in 4 days with acclimated sludge, it cannot be determined if this test substance is considered readily biodegradable by OECD criteria

Result :

The biological degradation of chlorophenols in activated sludge was studied. 2,5-Dichlorophenol was more resistent to degradation than 2,4-dichlorophenol. While 2,4-dichlorophenol was 100% degraded, including ring degradation, in five days, 2,5-dichlorophenol was only 52% ring-degraded in four days. [USEPA; Ambient Water Quality Criteria Doc: Chlorinated Phenols p.C-29 (1980) EPA 440/5-80-032]**PEER REVIEWED** As cited in HSDB record for 2,5-dichlorophenol, update of 8-09-200

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 2,5-Dichlorophenol CAS 583-79-8
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (2)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Ingols RS et al; J Water Pollut Control Fed 38: 629-35 (1966) As cited in HSDB update of 8-09-2001

(3) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

I U C L I D

Data Set

Existing Chemical	:	ID: 1984-58-3
CAS No.	:	1984-58-3
Generic name	:	2,5-dichloroanisole

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 21 °C
Sublimation	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)ccc(CL)c(OC)c1 CHEM : 2,5-Dichloroanisole MOL FOR: C7 H6 CL2 O1 MOL WT : 177.03 SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 215.67 deg C (Adapted Stein and Brown Method) Melting Point: 29.02 deg C (Adapted Joback Method) Melting Point: 12.27 deg C (Gold and Ogle Method) Mean Melt Pt : 20.65 deg C (Joback; Gold,Ogle Methods) Selected MP: 20.65 deg C (Mean Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-Dichloroanisole CAS 1984-58-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

2.2 BOILING POINT

Value	:	ca. 216 °C at 1013 hPa
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)ccc(CL)c(OC)c1 CHEM : 2,5-Dichloroanisole MOL FOR: C7 H6 CL2 O1 MOL WT : 177.03 SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 215.67 deg C (Adapted Stein and Brown Method)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-Dichloroanisole CAS 1984-58-3
Reliability	:	(2) valid with restrictions

Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.4 VAPOUR PRESSURE

Value : ca. .22 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year : 2001
GLP : no
Test substance :

Method : Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result : MPBPWIN (v1.40) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : c1(CL)ccc(CL)c(OC)c1
CHEM : 2,5-Dichloroanisole
MOL FOR: C7 H6 CL2 O1
MOL WT : 177.03

- SUMMARY MPBPWIN v1.40 ----------

Vapor Pressure Estimations (25 deg C):
(Using BP: 215.67 deg C (estimated))
(MP not used for liquids)
VP: 0.176 mm Hg (Antoine Method)
VP: 0.152 mm Hg (Modified Grain Method)
VP: 0.253 mm Hg (Mackay Method)
Selected VP: 0.164 mm Hg (Mean of Antoine & Grain methods)
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 2,5-Dichloroanisole CAS 1984-58-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. 3.36 at 25 °C
pH value :
Method :
Year : 2001
GLP : no
Test substance :

Method : Estimation using KOWWIN v1.66 in EPIWIN 3.05
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 2,5-Dichloroanisole CAS 1984-58-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	ca. 75 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05

Result : Water Sol from Kow (WSKOW v1.40) Results:

==========

Water Sol: 76.44 mg/L

SMILES : c1(CL)ccc(CL)c(OC)c1
CHEM : 2,5-Dichloroanisole
MOL FOR: C7 H6 CL2 O1
MOL WT : 177.03

- WSKOW v1.40 Results ----------

Log Kow (estimated) : 3.36
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 3.36

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -3.365
Water Solubility at 25 deg C (mg/L): 76.44

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	2,5-Dichloroanisole CAS 1984-58-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000
Rate constant	:	cm^3/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	
Test substance	:	

Method : Estimation using APOWIN v1.90 in EPIWIN 3.05

Result :
AOP Program (v1.90) Results:
==========
SMILES : c1(CL)ccc(CL)c(OC)c1
CHEM : 2,5-Dichloroanisole
MOL FOR: C7 H6 CL2 O1
MOL WT : 177.03

- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.8296 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 4.4167 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 5.2463 E-12 cm3/molecule-sec
HALF-LIFE = 2.039 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 24.465 Hrs

Source : Toxicology and Regulatory Affairs Flemington NJ

Test substance : 2,5-Dichloroanisole CAS 1984-58-3

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

26.12.2001 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	

Method : Estimated on chemical principles based on absence of groups susceptible to hydrolysis

Remark : The estimation program in EPIWIN has no capability to

estimate hydrolysis rates for this compound

Result : This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.

Source : Toxicology and Regulatory Affairs Flemington NJ

Test substance : 2,5-Dichloroanisole CAS 1984-58-3

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

26.12.2001 (2)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media :

Air :

Water :

Soil :

Biota :

Soil :

Method :

Year : 2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the EPIWIN derived estimates that were assessed for reasonableness compared with similar compounds. Half life in air was determined from the APOWIN program for 2,5-dichlorophenol as this would be the likely volatile species. Direct photolysis was not considered in this model. Emissions were calculated from air water and soil as this test substance it is volatile. Other parameters used the default values found in EPIWIN

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : 2,5-Dichloroanisole
  Molecular Wt: 177.03
  Henry's LC  : 0.00315 atm-m3/mole (Henrywin program)
  Vapor Press : 0.164 mm Hg  (Mpbpwin program)
  Log Kow     : 3.36  (Kowwin program)
  Soil Koc    : 939  (calc by model)

           Concentration   Half-Life    Emissions
             (percent)        (hr)       (kg/hr)
   Air       7.6             48.9         1000
   Water     22.8            900          1000
   Soil      68.8            900          1000
   Sediment  0.812           3.6e+003     0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
Air       1.14e-010    1.16e+003   823          38.8        27.4
Water     2.19e-008    190         247          6.34        8.23
Soil      3.22e-008    573         0            19.1        0
Sediment  1.66e-008    1.69        0.176        0.0564      0.00586


   Persistence Time: 361 hr
   Reaction Time:    561 hr
   Advection Time:   1.01e+003 hr
   Percent Reacted:  64.3
   Percent Advected: 35.7

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      48.94
      Water:    900
      Soil:     900
      Sediment: 3600
        Biowin estimate: 2.337  (weeks-months)
```

```
Advection Times (hr):
   Air:       100
   Water:     1000
   Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 2,5-Dichloroanisole CAS 1984-58-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (1)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

I U C L I D

Data Set

Existing Chemical	:	ID: 63734-62-3
CAS No.	:	63734-62-3
Generic name	:	benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy]

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	19.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 146 °C
Sublimation	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)O)c2 CHEM : Trifluorobenzoic acid CAS 63734-62-3 MOL FOR: C14 H8 CL1 F3 O3 MOL WT : 316.67 SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 387.24 deg C (Adapted Stein and Brown Method) Melting Point: 281.72 deg C (Adapted Joback Method) Melting Point: 112.45 deg C (Gold and Ogle Method) Mean Melt Pt : 197.08 deg C (Joback; Gold,Ogle Methods) Selected MP: 146.30 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid CAS 63734-62-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

27.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	= .0000029 hPa at °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)O)c2 CHEM : Trifluorobenzoic acid CAS 63734-62-3 MOL FOR: C14 H8 CL1 F3 O3 MOL WT : 316.67

SUMMARY MPBPWIN v1.40 ----------

Vapor Pressure Estimations (25 deg C):
(Using BP: 387.24 deg C (estimated))
(Using MP: 146.30 deg C (estimated))
VP: 2.66E-007 mm Hg (Antoine Method)
VP: 9.96E-007 mm Hg (Modified Grain Method)
VP: 2.18E-006 mm Hg (Mackay Method)
Selected VP: 9.96E-007 mm Hg (Modified Grain Method)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid CAS 63734-62-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. 4.7 at 25 °C
pH value :
Method :
Year : 2001
GLP : no
Test substance :

Method : Estimation using KOWWIN v1.66 in EPIWIN 3.05
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid CAS 63734-62-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 1 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method :
Year : 2001
GLP : no
Test substance :

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05
Result : Water Sol from Kow (WSKOW v1.40) Results:
==========

Water Sol: 0.9521 mg/L

SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)O)c2
CHEM : Trifluorobenzoic acid CAS 63734-62-3
MOL FOR: C14 H8 CL1 F3 O3
MOL WT : 316.67

- WSKOW v1.40 Results ----------

Log Kow (estimated) : 4.70
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 4.70

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
Acid, aromatic	0.000

Log Water Solubility (in moles/L) : -5.522
Water Solubility at 25 deg C (mg/L): 0.9521

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : 3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid CAS 63734-62-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000
Rate constant	:	cm^3/(molecule*sec)
Degradation	:	% after
Method	:	Estimation using APOWIN v1.90 in EPIWIN 3.05
Result	:	AOP Program (v1.90) Results: ========== SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)O)c2 CHEM : Trifluorobenzoic acid CAS 63734-62-3 MOL FOR: C14 H8 CL1 F3 O3 MOL WT : 316.67 - SUMMARY (AOP v1.90): HYDROXYL RADICALS -- Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.5200 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec **Addition to Aromatic Rings = 1.3056 E-12 cm3/molecule-sec Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec OVERALL OH Rate Constant = 1.8256 E-12 cm3/molecule-sec HALF-LIFE = 5.859 Days (12-hr day; 1.5E6 OH/cm3) HALF-LIFE = 70.306 Hrs ** Designates Estimation(s) Using ASSUMED Value(s)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid CAS 63734-62-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

27.12.2001 (1)

3.1.2 STABILITY IN WATER

Type	:	
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark	:	The estimation program in EPIWIN has no capability to

estimate hydrolysis rates for this compound.

Result : This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.

Source : Toxicology and Regulatory Affairs Flemington NJ

Test substance : 3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid CAS 63734-62-3

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

27.12.2001 (2)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media :

Air :

Water :

Soil :

Biota :

Soil :

Method :

Year : 2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the EPIWIN derived estimates (Biowin, Ultimate) that were assessed for reasonableness compared with similar compounds. Half life in air was determined from the APOWIN program. Direct photolysis was not considered in this model. Emissions were calculated from only water and soil as this test substance it is almost non volatile. Other parameters used the default values found in EPIWIN.

Result :

```
======================================
  Chem Name   : Trifluorobenzoic acid CAS 63734-62-3
  Molecular Wt: 316.67
  Henry's LC  : 1.53e-008 atm-m3/mole (Henrywin program)
  Vapor Press : 9.96e-007 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.58e-005 mm Hg  (super-cooled)
  Melting Pt  : 146 deg C (Mpbpwin program)
  Log Kow     : 4.7  (Kowwin program)
  Soil Koc    : 2.05e+004  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
  Air       2.57e-005       141          0
  Water     19              1.44e+003    1000
  Soil      63.4            1.44e+003    1000
  Sediment  17.7            5.76e+003    0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
Air       6.15e-016    0.00415     0.00842     0.000207    0.000421
Water     1.45e-013    299         621         14.9        31.1
Soil      1.13e-014    999         0           49.9        0
Sediment  1.41e-013    69.6        11.6        3.48        0.578

   Persistence Time: 1.64e+003 hr
   Reaction Time:    2.4e+003 hr
   Advection Time:   5.18e+003 hr
   Percent Reacted:  68.4
   Percent Advected: 31.6

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      140.6
      Water:    1440
      Soil:     1440
      Sediment: 5760
        Biowin estimate: 1.810  (months      )
```

```
Advection Times (hr):
   Air:       100
   Water:     1000
   Sediment: 5e+004
```

Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid CAS 63734-62-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

27.12.2001 (1)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
NOEC	:	180
LC50	:	> 1000
Method	:	other: EPA
Year	:	1975
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS
- Species: Lepomis macrochirus Rafinesque
- Supplier: commercial hatchery in Nebraska
- Age;size;weight;loading: ~4 months; 28-44 mm; 0.20-1.10 g; 0.3-0.4 g/L
- Feeding during test: none, feeding was discontinued 48 hours prior to test initiation

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none
- Other procedures: direct addition of the test substance to the test vessels

DILUTION WATER
- Source: Well water (Tarrytown site)
- Chemistry (Alkalinity 32 mg CaCO3/L;Hardness 46 mg CaCO3/L/pH 7.70/Conductance 150 umhos/cm)

TEST SYSTEM
- Test type: static
- Concentrations: 0, 100, 180, 320, 560 and 1000 mg/L
- Exposure vessel type: 20 L glass vessels containing 15 L of water
- Number of fish: 10 per treatment
- Photoperiod: not indicated

PHYSICAL MEASUREMENTS
- Measuring times: 0, 48, 96 hours
- Test temperature: 22-23 C
- Dissolved oxygen: 61-101%
- pH: 7.3-7.7

DURATION OF THE TEST: 96 hours

TEST PARAMETER: mortality/symptoms
OBSERVATION TIMES: daily

STATISTICAL METHOD: not indicated

Result : RESULTS:
- Mortality: no mortality
- Other effects: irritated, exhibited abnormal sounding behaviour and/or dark discolouration at 320-1000 mg/L.

REFERENCE SUBSTANCE: 96 h LC50 4.03 ug/L (3.59-4.52 ug/L)

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 63734-62-3: TD 77-373 (RH-41,833 W. Liq. (2.6

eq.)), purity not indicated

Reliability : (2) valid with restrictions
1. No analyses were performed to confirm the nominal test concentrations. The study reliability was lowered because of this.
2. Fish were fasted longer than recommended (48 h, OECD 203 24 h). This may have increased the susceptibility of the fish.
3. The used fish were larger than recommended by the guideline of the OECD, but acceptable according to the EG-guideline (28-44 mm, OECD 20+/-10 mm, EG 50+/-20 mm).
4. The test substance was specified as TD 77-373 (RH-41,833 W. Liq. (2.6 eq.)). No information was available on the composition of this compound.

09.05.2001 (8)

Type : static
Species : Lepomis macrochirus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : 180
LC50 : > 1000
Limit test :
Analytical monitoring : no data
Method : other: EPA 660/3-75-009
Year : 1975
GLP : no
Test substance : other TS

Method : TEST ORGANISMS
- Species: Lepomis macrochirus Rafinesque
- Supplier: commercial hatchery in Nebraska
- Age;size;weight;loading: ~4 months; ? mm; ~0.68-0.78 g; 0.5 g/L
- Feeding during test: none, feeding was discontinued 48 hours prior to test initiation

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none
- Other procedures: direct addition of the test substance to the test vessels

DILUTION WATER
- Source: Well water (Tarrytown site)
- Chemistry (Alkalinity 32 mg CaCO3/L;Hardness 46 mg CaCO3/L/pH 7.56/Conductance 150 umhos/cm)

TEST SYSTEM
- Test type: static
- Concentrations: 0, 100, 180, 320, 560 and 1000 mg/L
- Exposure vessel type: 20 L glass vessels containing 15 L of water
- Number of fish: 10 per treatment
- Photoperiod: not indicated

PHYSICAL MEASUREMENTS
- Measuring times: 0, 48, 96 hours at control, low, middle and high dose
- Test temperature: 22-23 C
- Dissolved oxygen:
Control: 101/61/56 at respectively 0/24/48 h
100 mg/L: 99/47/45 at respectively 0/24/48 h
320 & 1000 mg/L: 100/20/16-18 at respectively 0/24/48 h

- pH: 6.6-7.7

DURATION OF THE TEST: 96 hours

TEST PARAMETER: mortality/symptoms
OBSERVATION TIMES: daily

REFERENCE SUBSTANCE: p,p'-DDT

STATISTICAL METHOD: not indicated

Result : RESULTS:
- Mortality: no mortality
- Other effects: quiescence, abnormal surfacing, erratic swimming and/or gulping of air at 320-1000 mg/L.

REFERENCE SUBSTANCE: 96 h LC50 4.03 ug/L (3.59-4.52 ug/L)

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 63734-62-3: TD 77-370 (RH-41,833 HOAc ppt (2.6 eq.)), purity not indicated

Reliability : (2) valid with restrictions
1. No analyses were performed to confirm the nominal test concentrations. The study reliability was lowered because of this.
2. The oxygen concentrations dropped to minimal 16% at the end of the test (OECD 203 >60%). Further the fish were fasted longer than recommended (48 h, OECD 203 24 h). Both factors may have increased the susceptibility of the fish.
3. There was no information on the length of the test organisms, since table 3 of the report (containing this information) was missing.
4. The test substance was specified as TD 77-370 (RH-41,833 HOAc ppt (2.6 eq.)). No information was available on the composition of this compound.

09.05.2001 (7)

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : 1.4
LC50 : 2.6
Limit test :
Analytical monitoring : no data
Method : other: EPA 660/3-75-009
Year : 1975
GLP : no
Test substance : other TS

Method : TEST ORGANISMS
- Species: Pimephales promelas
- Supplier: commercial fish farmer in Arkansas
- Size;weight;loading: 44+/-3.9 mm;0.75+/-0.30 g;0.5 g/L
- Feeding during test: not fed (feeding was discontinued 48 hours prior to the test

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: acetone

DILUTION WATER
- Source: Well water
- Chemistry (Alkalinity/Hardness 35 mg CaCO3/L/pH 7.1)

TEST SYSTEM
- Test type: static
- Concentrations: 0 (untr), 0 (veh), 1.4, 1.8, 2.4, 3.2, 4.2, 6.5, 10, 18 mg/L
- Exposure vessel type: 20 L glass vessel containing 15 L of test solution
- Number of fish: 10 per treatment
- Photoperiod: not indicated
PHYSICAL MEASUREMENTS
- Measuring times: 0, 24, 48, 96 hours
- Test temperature: 22+/-1 C
- Dissolved oxygen: decreased from 100% (0 h) to 25% (96 h)
- pH: 6.8-7.2

DURATION OF THE TEST: 96 hours

TEST PARAMETER: mortality/symptoms
OBSERVATION TIMES: 24, 48, 96 hours

STATISTICAL METHOD: least square regression analysis

Result : RESULTS:
- Nominal concentrations (mg/L): 0 (untr),) (veh), 1.4, 1.8, 2.4, 3.2, 4.2, 6.5, 10 and 18
- Mortality [%]: 0, 0, 0, 60, 50, 40, 90, 100, 100, 100
- Other effects: dark discoloured, lethargic, loss of equilibrium and/or expired in test concentrations from 1.8 mg/L
- Concentration / response curve: yes
- Effect concentration vs. test substance solubility: In test concentrations from 2.4 mg/L a crystalline precipitate was observed. This precipitate disappeared almost completely within 24 hours, except for the highest test concentration (18 mg/L).

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 63734-62-3 (RH-41,833), purity not indicated

Conclusion : 96 h LC50 2.6 mg/L (95% CI 2.0-3.3 mg/L)
96 h NOEC 1.4 mg/L

Reliability : (2) valid with restrictions
1. No analyses were performed to confirm the nominal test concentrations. Since also undissolved substance was reported, tha actual test concentrations may have been lower. The study reliability was lowered because of this.
2. The oxygen concentrations dropped to 25% at the end of the test (OECD 203 >60%). Further the fish were fasted longer than recommended (48 h, OECD 203 24 h). Both factors may have increased the susceptibility of the fish.
3. The used fish were larger than recommended by the guideline of the OECD, but acceptable accoring to the EG-guideline (44+/-4 mm, OECD 20+/-10 mm, EG 50+/-20 mm).

09.05.2001 (5)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1170 mg/kg bw
Species	:	rat
Strain	:	other: CF Nelson
Sex	:	male
Number of animals	:	5
Vehicle	:	other: oil
Doses	:	
Method	:	other: not indicated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: not indicated - Age: not indicated - Number: 5/dose - Weight at study initiation: 189-199 g (mean) - Controls: no ADMINISTRATION: - Doses: 625, 1250 and 2500 mg/kg bw - Doses per time period: single - concentration: 20% w/v - Post dose observation period: 14 days - food withheld for 24 hours pre-dosing EXAMINATIONS: signs for toxicity and gross necropsy BODY WEIGHT: pre-dosing and at termination of study STATISTICAL METHOD: not indicated
Result	:	MORTALITY: - Number of deaths at each dose: 625, 1250 and 2500 mg/kg bw: 0/5, 3/5 and 5/5, respectively - Time of death: for the highest dose: within 24 hours; for 1250 mg/kg bw: within 4 days CLINICAL SIGNS: lethargy, prostration at 2500 mg/kg bw (0-6 hours) BODY WEIGHT: survivors increased bw NECROPSY FINDINGS: survivors normal, at 2500 mg/kg decendents were normal, at 1250 mg/kg one decendent had blood in small intestines.
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	III, 63734-62-3 (3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid), purity 86.5%, used as 20% dispersion with oil
Conclusion	:	LD50 1170 mg/kg bw
Reliability	:	(2) valid with restrictions 1. The information available in the report on the study findings is essentially confined to what is included in the above summary. There is no information on the individual

toxicity data.
2. The study is not reliable because the LD50 cannot be back-calculated to the amount of a.i./kg body weight (dosing was done with a 20% weight/volume oil dispersion and no data are available on the density of the oil).

19.02.2003 (3)

Type	:	LD50
Value	:	> 50 mg/kg bw
Species	:	rat
Strain	:	other: Charles River CD
Sex	:	male
Number of animals	:	6
Vehicle	:	other: 0.5% methylcellulose in water solution
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: not indicated
- Age: not indicated
- Number: 6/dose
- Weight at study initiation: 227-230 g
- Controls: no

ADMINISTRATION:
- Doses: 50 and 500 mg/kg bw
- Doses per time period: single
- concentration: 10% w/v
- Post dose observation period: 14 days
- food withheld for 24 hours pre-dosing

EXAMINATIONS: signs for toxicity and gross necropsy

BODY WEIGHT: pre-dosing and at termination of study

STATISTICAL METHOD: not indicated

Result :

MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: lethargy, ataxia at both doses

BODY WEIGHT: no effects

NECROPSY FINDINGS: no visible lesions

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	III, 63734-62-3 (3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid), purity 97%, used as 10% (w/v) dispersion
Conclusion	:	LD50 > 500 mg/kg bw (> 50 mg a.i./kg bw)
Reliability	:	(2) valid with restrictions 1. The information available in the report on the study findings is essentially confined to what is included in the above summary. There is no information on the individual toxicity data. 2. The LD50 is back-calculated to the amount of a.i./kg body weight (dosing was done with a 10% weight/volume dispersion of 0.5% methylcellulose in water) using a density of about 1 g/ml.

10.04.2001 (4)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 3.4 mg/l
Species	:	rat
Strain	:	other: Crl:CD(SD)BR
Sex	:	male/female
Number of animals	:	24
Vehicle	:	other: none
Doses	:	
Exposure time	:	4 hour(s)
Method	:	other: not specified
Year	:	
GLP	:	yes
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: Charles River Breeding Laboraties (Portage, MI)
- Age: not specified
- Weight at study initiation: not included in the report
- Number of animals: 12/sex/dose
- Controls: yes (12/sex)

ADMINISTRATION:
- Type of exposure: whole body exposure to test substance dust
- Exposure duration: 4 hours
- Half of the rats (6m/6f) were killed immediately after exposure, the other half on day 14 post-exposure
- Type or preparation of particles: with dust generator
- Air changes: 15/hour

EXAMINATIONS: for toxic signs once every hour during exposure and twice daily during the post-exposure period.
- Haematology: hemoglobin, hematocrit, red cell count, white cell count, clot time, platelet count, prothrobin time, partial tromboplastin time and activated partial thromboplastin time.
- Necropsy for macroscopic abnormalities of organs (cervical lymph nodes, salivary glands, thyroids, trachea, lungs, heart and aorta, thymus, liver, stomach, nasal turbinates, pancreas, spleen, intestines, kidneys, adrenals, bladder, testes/ovaries, uterus and eyes).
- Those organs which showed abnormalities were examined histopathologically (trachea, lungs and nasal turbinates).

BODY WEIGHT: on days 0 (pre-dosing), 1, 3, 5, 7, 11, and 14

ANALYSES: chamber analytical concentration and particle size distribution
- Method: gravimetry
- Sampling times: analytical concentration: no data, PSD: twice (110 and 197 min)
- Concentrations(nominal/measured): 102.46 mg/l / 3.39 +/- 0.56 mg/l (n=13)
- Particle size: mass median diameter of 9.0 (+/- 1.8) and 8.5 (+/- 1.8) microns at 110 and 197 minutes into the exposure, resp.

STATISTICAL METHOD: PSD by log-probit regression analysis (Hagan, 1980)

Result : MORTALITY:
- Number of deaths at each dose: no deaths in the control
2 deaths in the dose group
- Time of death: 2 days post-exposure

CLINICAL SIGNS: during exposure of treated animals: dyspnea, gasping, eye squint, lacrimation, salivation, red exudate around the eyes.
post-exposure of treated animals: thriftless appearance, red exudates around the eyes and muzzle, yellow-stained anal-genital area, alopecia around the eyes and muzzle, ptosis, exophthalmus, corneal opacities, lacrimation, nasal discharge, dyspnea, rales, ataxia, decreased motor activity, and prostration.

BODY WEIGHT: control animals no body weight losses
treated animals: body weight losses on day 1 and 2, followed by body weight gains on day 7 to 11.

HEMATOLOGY: reduced white blood cell counts and increased platelet counts.

NECROPSY FINDINGS: control group: no gross lesions (8M,9F), hardened and/or enlarged salivary glands (4M,1F), hardened and/or enlarged cervical lymph nodes (2M,1F), diffuse brown areas on the lung (1M,1F), and dilated kidney medulla (1M).
treated group: decendents: redness of lungs (2F), yellow-stained anal-genital area (2F), and red-stained muzzle (2F); surviving animals (0 and 14 days): no gross lesions (4M,5F), corneal opacities (6M,2F), red-spotted cervical lymph nodes (1F), hardened salivary glands (1F), dilated kidney medulla (1M) and alopecia around the eyes (1F).
Histopathology reveals degeneration of the respiratory and olfactory epithelium and congestion of the mucosa of the nasal cavity.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, 63734-62-3
(3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid), purity 100%

Conclusion : LC50 > 3.4 mg/l

Reliability : (3) invalid
1. This report did not contain tables, nor figures. So, no individual data were present.
2. There is a great difference in nominal versus measured concentration of the test substance dust.
3. The study is not reliable because all animals showed a viral infection "Sialodacryoadenitis (SDA)" during the test. The interpretation of in-life observations is complicated by this fact and especially the hematology is obscured.
4. Due to the use of an out-of-date lot of Vacutainer tubes, the determination of the coagulation parameters was prevented.

10.04.2001 (9)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> 5000 mg/kg bw
Species	:	rabbit
Strain	:	other: Albino
Sex	:	male
Number of animals	:	5
Vehicle	:	water
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: not indicated - Age: not indicated - Weight at study initiation: 2.23-2.32 kg (mean) - Controls: no ADMINISTRATION: - Area covered: not specified - Occlusion: yes - Vehicle: aqueous paste - Concentration in vehicle: not specified - Doses: 2500 and 5000 mg/kg bw - Removal of test substance: no data - contact time: 24 hours EXAMINATIONS: signs of intoxication, skin irritation and gross autopsy BODY WEIGHT: pre-dosing and at end of the test STATISTICAL METHOD: no data
Result	:	MORTALITY: - Number of deaths at each dose: 2500 and 5000 mg/kg bw: 0/5 and 1/5, respectively - Time of death: between days 8 and 14 CLINICAL SIGNS: no signs of intoxication, very slight erythema, no edema observed BODY WEIGHT: normal NECROPSY FINDINGS: normal in both decendents and survivors
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	III, 63734-62-3 (3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid), purity 86.5%, aqueous paste
Conclusion	:	LD50 > 5000 mg/kg bw
Reliability	:	(4) not assignable 1. The information was essentially confined to what is included in the current summary. No data were present on body area covered, concentration a.i. in the paste. This lowers the reliability of the study. 2. only males are included

10.04.2001 (3)

Type	:	LD50
Value	:	> 200 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male
Number of animals	:	6
Vehicle	:	physiol. saline
Doses	:	
Method	:	other: not specified
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: not indicated
- Age: not indicated
- Weight at study initiation: 2.76 kg (mean)
- Controls: no

ADMINISTRATION:
- Area covered: not specified
- Occlusion: yes
- Vehicle: paste with saline
- Concentration in vehicle: not specified
- Doses: 200 mg/kg bw
- Removal of test substance: no data
- contact time: 24 hours

EXAMINATIONS: signs of intoxication, skin irritation and gross autopsy

BODY WEIGHT: pre-dosing and at end of the test

STATISTICAL METHOD: no data

Result :

MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: no signs of intoxication; no skin irritation observed on the intact skin; well defined erythema and slight edema observed on abraded skin.

BODY WEIGHT: normal

NECROPSY FINDINGS: no visible lesions; 1 rabbit indentation in surface of kidneys

Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	III, 63734-62-3 (3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid), purity 97%, used as saline paste
Conclusion	:	LD50 > 200 mg/kg bw
Reliability	:	(4) not assignable 1. The information was essentially confined to what is included in the current summary. No data were present on body area covered, concentration a.i. in the paste. This lowers the reliability of the study. 2. Abrasion of the skin can influence the permeability of the test substance.

10.04.2001 (4)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	TA1535, TA1537, TA98 and TA100
Test concentration	:	75-7500 ug/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	SYSTEM OF TESTING: - Species/cell type: Salmonella typhimurium TA98, TA100, TA1535, TA1537. - Deficiences/Proficiences: histidine - Metabolic activation system: rat S9 mix (Arochlor 1254 induced) ADMINISTRATION: - Dosing: 0, 75, 250, 750, 2500, 7500µg/plate - Number of replicates: unknown - Application: DMSO or saline buffer - Positive and negative control groups and treatment: Positive controls: ±S-9: 2-anthramine for TA1535, TA1537 and TA100, ±S-9 2-Acetaminofluorene for TA98. Negative controls: DMSO - type of test: no data
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 63734-62-3, (3-(2-chloro-4-trifluoromethylphenoxy)benzoic acid), purity 88.5%
Reliability	:	(4) not assignable 1. The information given in the report was essentially confined to what is included in the current summary. 2. No strain with an AT basepair at the primary reversion site is tested.

17.05.2001 (6)

5.6 GENETIC TOXICITY 'IN VIVO'

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(3) Rohm & Haas Co, Acute toxicity studies with 3-(2-chloro-4-(trifluoromethyl)phenoxy)benzoic acid in rats and rabbits, 1976 (48)

(4) Rohm & Haas Co, Acute toxicity studies with 3-(2-chloro-4-(trifluoromethyl)phenoxy)benzoic acid in rats and rabbits, 1978 (49)

(5) Rohm and Haas Company, Acute toxicity of RH-41,833 to fathead minnow (Pimephales promelas), 1976 (47)

(6) Rohm and Haas Company, RH-41, 833 microbial mutagen test (final report) with cover letter dated 07.17.84

(7) Rohm and Haas Company, The acute toxicity of TD-77-370 to Bluegill sunfish, 1978 (52)

(8) Rohm and Haas Company, The acute toxicity of TD-77-373 to the Bluegill sunfish Lepomis macrochirus Rafinesque, 1978 (50)

(9) Rohm and Haas Company, Toxicology Department, Acute Inhalation Toxicity Study in Rats, 1985 (46)

I U C L I D

Data Set

Existing Chemical	:	ID: 72252-48-3
CAS No.	:	72252-48-3
Generic name	:	Benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy], potassium salt

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	21.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	ca. 251 °C
Sublimation	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)OK)c2 CHEM : Potassium Trifluorobenzoic acid CAS 72252-48-3 MOL FOR: C14 H7 CL1 F3 O3 K1 MOL WT : 354.76 - SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 583.20 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 226.87 deg C (Gold and Ogle Method) Mean Melt Pt : 288.36 deg C (Joback; Gold,Ogle Methods) Selected MP: 251.47 deg C (Weighted Value)
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	Potassium salt of benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy CAS 72252-48-3
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

27.12.2001 (1)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .000000001 hPa at °C
Decomposition	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	
Method	:	Estimation using MPBPWIN v1.40 in EPIWIN 3.05
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)OK)c2 CHEM : Potassium Trifluorobenzoic acid CAS 72252-48-3 MOL FOR: C14 H7 CL1 F3 O3 K1

MOL WT : 354.76

- SUMMARY MPBPWIN v1.40 ----------

Vapor Pressure Estimations (25 deg C):
(Using BP: 583.20 deg C (estimated))
(Using MP: 251.47 deg C (estimated))
VP: 2.57E-016 mm Hg (Antoine Method)
VP: 6.93E-013 mm Hg (Modified Grain Method)
VP: 2.46E-012 mm Hg (Mackay Method)

Selected VP: 6.93E-013 mm Hg (Modified Grain Method

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium salt of benzoic acid,
3-[2-chloro-4-(trifluoromethyl)phenoxy CAS 72252-48-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

2.5 PARTITION COEFFICIENT

Partition coefficient :
Log pow : ca. .56 at °C
pH value :
Method :
Year : 2001
GLP : no
Test substance :

Method : Estimation using KOWWIN v1.66 in EPIWIN 3.05
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium salt of benzoic acid,
3-[2-chloro-4-(trifluoromethyl)phenoxy CAS 72252-48-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 1900 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method :
Year : 2001
GLP : no
Test substance :

Method : Estimation using WSKOW v1.40 in EPIWIN 3.05
Result : Water Sol from Kow (WSKOW v1.40) Results:
==========

Water Sol: 1946 mg/L

SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)OK)c2
CHEM : Potassium Trifluorobenzoic acid CAS 72252-48-3
MOL FOR: C14 H7 CL1 F3 O3 K1
MOL WT : 354.76

- WSKOW v1.40 Results ----------

Log Kow (estimated) : 0.56
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 0.56

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s):	Value
No Applicable Correction Factors	

Log Water Solubility (in moles/L) : -2.261
Water Solubility at 25 deg C (mg/L): 1946

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium salt of benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy CAS 72252-48-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000
Rate constant	:	cm^3/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	
Test substance	:	

Method : Estimation using APOWIN v1.90 in EPIWIN 3.05
Remark : Due to the low volatility, this reaction unlikely in practice.
Result : AOP Program (v1.90) Results:

==========

SMILES : c1(CL)cc(C(F)(F)(F))ccc1Oc2cccc(C(=O)OK)c2
CHEM : Potassium Trifluorobenzoic acid CAS 72252-48-3
MOL FOR: C14 H7 CL1 F3 O3 K1
MOL WT : 354.76

- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------

Hydrogen Abstraction = 0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.8598 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 1.8598 E-12 cm3/molecule-sec
HALF-LIFE = 5.751 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 69.012 Hrs

.. ** Designates Estimation(s) Using ASSUMED Value(s)

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium salt of benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy CAS 72252-48-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 °C
t1/2 pH7	:	> 1 year at 25 °C
t1/2 pH9	:	> 1 year at 25 °C
Deg. product	:	
Method	:	

Year : 2001
GLP : no
Test substance :

Method : Estimated on chemical principles based on absence of groups susceptible to hydrolysis
Remark : The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.
Result : This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium salt of benzoic acid, 3-[2-chloro-4-(trifluoromethyl)phenoxy CAS 72252-48-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (2)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air :
Water :
Soil :
Biota :
Soil :
Method :
Year : 2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Estimated values were used for physical constants. Biodegradation was based on the EPIWIN derived estimates (Biowin, Ultimate) that were assessed for reasonableness compared with similar compounds. Half life in air was determined from the APOWIN program. Direct photolysis was not considered in this model. Emissions were calculated from only water and soil as this test substance it is non-volatile. Other parameters used the default values found in EPIWIN.

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Potassium Trifluorobenzoic acid CAS 72252-48-3
  Molecular Wt: 354.76
  Henry's LC  : 1.66e-016 atm-m3/mole (calc VP/Wsol)
  Vapor Press : 6.93e-013 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.2e-010 mm Hg  (super-cooled)
  Melting Pt  : 251 deg C (Mpbpwin program)
  Log Kow     : 0.56  (Kowwin program)
  Soil Koc    : 1.49  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.07e-014       138          0
   Water     58.4            3.6e+003     1000
   Soil      41.4            3.6e+003     1000
   Sediment  0.118           1.44e+004    0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
Air       2.55e-029    1.39e-012   2.76e-012   6.94e-014   1.38e-013
Water     3.53e-021    290         1.5e+003    14.5        75.2
Soil      8.27e-020    205         0           10.3        0
Sediment  3.44e-021    0.146       0.0607      0.00731     0.00304
```

```
Persistence Time: 1.29e+003 hr
Reaction Time:    5.2e+003 hr
Advection Time:   1.71e+003 hr
Percent Reacted:  24.8
Percent Advected: 75.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
   Air:      138
   Water:    3600
   Soil:     3600
   Sediment: 1.44e+004
     Biowin estimate: 1.638  (recalcitrant)

Advection Times (hr):
   Air:      100
   Water:    1000
   Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : Potassium salt of benzoic acid,
3-[2-chloro-4-(trifluoromethyl)phenoxy CAS 72252-48-3
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (1)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(2) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

I U C L I D

Data Set

Existing Chemical	:	ID: 50594-66-6
CAS No.	:	50594-66-6
Generic name	:	Acifluorfen

Producer Related Part

Company	:	Toxicology and Regulatory Affairs
Creation date	:	26.12.2001

Substance Related Part

Company	:	Toxicology and Regulatory Affairs
Creation date	:	26.12.2001
Memo	:	
Printing date	:	27.12.2001
Revision date	:	
Date of last Update	:	27.12.2001
Number of Pages	:	204
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.9 SOURCE OF EXPOSURE

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value	:	= 150 ° C
Sublimation	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	
Remark	:	Published data found in EPIWIN. SRC data base Supported by Estimation using MPBPWIN v1.40 in EPIWIN 3.05 - SUMMARY MPBPWIN v1.40 ---------- Boiling Point: 442.92 deg C (Adapted Stein and Brown Method) Melting Point: 349.84 deg C (Adapted Joback Method) Melting Point: 144.96 deg C (Gold and Ogle Method) Mean Melt Pt : 247.40 deg C (Joback; Gold,Ogle Methods) Selected MP: 185.94 deg C (Weighted Value)
Result	:	CAS Number : 050594-66-6 Chem Name : ACIFLUORFEN Mol Formula: C14H7ClF3NO5 Mol Weight : 361.66 Melting Pt : 150 deg C
Test substance	:	Acifluorfen CAS 50594-66-6
Reliability	:	(2) valid with restrictions Data from handbooks and standard reference sources assigned a 2
Flag	:	Critical study for SIDS endpoint

26.12.2001 (7)

2.2 BOILING POINT

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .00000002 hPa at 25° C
Decomposition	:	
Method		other (calculated)
Year	:	1985
GLP	:	no data
Test substance	:	

Remark : Published data found in EPIWIN. SRC data base

Result : Vapor Pressure:
Value : 1.53E-008 mm Hg
Temp : 25 deg C
Type : EST
Ref : NEELY,WB & BLAU,GE (1985)

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (7)

Value : ca. .000000052 hPa at 25° C
Decomposition :
Method other (calculated)
Year : 2001
GLP : no
Test substance :
Method : Estimation using MPBPWIN v1.40 in EPIWIN 3.05

Result : -- SUMMARY MPBPWIN v1.40 ----------

Vapor Pressure Estimations (25 deg C):
(Using BP: 442.92 deg C (estimated))
(Using MP: 150.00 deg C (exp database))
VP: 3.26E-009 mm Hg (Antoine Method)
VP: 3.94E-008 mm Hg (Modified Grain Method)
VP: 8.94E-008 mm Hg (Mackay Method)
Selected VP: 3.94E-008 mm Hg (Modified Grain Method)

Test substance : Acifluorfen CAS 50594-66-6
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (5)

2.5 PARTITION COEFFICIENT

Log pow : = 3.7 at ° C
Method
Year : 1992
GLP : no data
Test substance :
Result : Log P (octanol-water):
Value : 3.70
Type : EXP
Ref : NANDIHALLI UB ET AL. (1992)

Test substance : Acifluorfen CAS 50594-66-6
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (7)

2.6.1 WATER SOLUBILITY

Value	:	= 120 mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	at and ° C
Method	:	
Year	:	1994
GLP	:	no data
Test substance	:	
Result	:	Water Solubility: Value : 120 mg/L Temp : 25 deg C Type : EXP Ref : TOMLIN,C (1994)
Test substance	:	Acifluorfen CAS 50594-66-6
Reliability	:	(2) valid with restrictions Published value
Flag	:	Critical study for SIDS endpoint

26.12.2001 (7)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Xenon lamp
Light spect.	:	> 290 nm
Rel. intensity	:	based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Deg. Product	:	
Method	:	EPA Guide-line subdivision N 161-2 "Photodegradation studies in water"
Year	:	
GLP	:	yes
Test substance	:	other TS

Method :

Photolysis of acifluorfen 14C-labelled in the nitrobenzoate moiety {5-[2-chloro-4-(trifluoro-methyl)-phenoxy]-2-nitro benzoic acid-UL-14C (N-label)} and in the phenoxy trifluoromethyl moiety {5-[2-chloro-4-(trifluoro-methyl)-phenoxy-UL-14C]-2-nitro benzoic acid (F-label)} was studied at 25 deg C. Hereto, TS (N- or F-label) was dissolved in sterile 0.025M phosphate buffer (1% acetonitrile) at concentrations in the range 4 - 5 ppm.
Volatiles were trapped in ethylene glycol (1 trap), 0.1N sulfuric (1 trap) acid and 1N NaOH (2 traps). Light source was a xenon lamp of intensity 1900 uE.m-2.s-1 (equivalent to summer noon time sun). Radiation < 290 nm was filtered out. Quantitation and identification/characterization was performed using LSC, TLC (two solvent systems), UV-vis spectroscopy and HPLC with 14C-detection (quantitation by scintillation of the column effluent). Intermediates and reference substances were derivatized by methylation using diazomethane and compared by 2D-HPLC.

The following reference substances were available:
Acifluorfen Amine
Desnitro acifluorfen
Acifluorfen Acid Amine
Acifluorfen Methyl Ester
Descarboxy Acifluorfen
Acifluorfen Acetamide
Amino Acifluorfen ME
Acifluorfen Amine Derivative
14C N-hexadecane
4-Nitrophenol
2-Nitrobenzoic acid
Anthranilic Acid
Acifluorfen

Dark controls and adsorption controls were included.

Samples were taken in N-label test mixture at 0, 0.94, 1.8, 3.8, 18.0, 22.4, 30.2, 41.7, 64.3, 70.0, 87.1, 92.7, 110.7, 111.8, 116.1, 134.4, 134.5, 140.3, 157.8, 158.0, 162.8, 182.0 and 204.5 hrs. Samples in F-label test mixture were taken at 0, 64.3, 87.1, 110.7, 134.5 and 158 hrs; dark

controls at 0, 64.3 and 110.7 hrs.

Result : Degradation could be described by 1st order kinetics; half lives measured for N-label TS were in the range 78-100 hrs, half-life measured for F-label TS was 95 (conc. 4-5 ppm).
% degradation N-label TS at 205 hrs: 81.4%
% degradation F-label TS at 158 hrs: 70.4%

Maximal concentration of metabolites (% of applied radioactivity) measured during irradiation period:

Meta-bolite*	N-label test mixture Max. % of applied	F-label test mixture Max. % of applied
P1	35.4	24.0
P2	5.1	7.4
P3	7.8	5.3
P4	6.8	5.6
P11	1.6	1.9
P12	1.8	1.6
Volatiles	0.2	3.3
	0.0	0.0 (Sulf. acid)
	9.4	5.1 (NaOH)

Remarks:
Concentration range (N-label): 4.42-4.86 ppm
Concentration (F-label): 3.98 ppm
Irradiation period: 205 hrs (N-label); 158 hrs (F-label)
Mass balance: 85.6-101.6%.

- Hydrolysis of volatile recovered in ethylene glycol yielded one major intermediate and one final moiety with an HPLC retention time identical to that of the compound trapped in NaOH. This suggests that the volatile in the NaOH trap is the hydrolysis product of the volatile incompletely trapped in ethylene glycol.
- Metabolites could not be identified. Based on reverse isotope dilution experiments formation of 2-nitrobenzoic acid and anthranilic acid could be excluded. Methylation did not yield distinct reaction products.
- Major metabolite (P1) appears to actually consist of a complex mixture of compounds (TLC and derivatization).
- No adsorption or degradation in dark control were observed.

Test substance : III, CAS 50594-66-6 (acifluorfen), actually 5-[2-chloro-4-(trifluoro-methyl)-phenoxy-UL-14C]-2-nitro benzoic acid, radiopurity 95.27% (HPLC)
III, CAS 50594-66-6 (acifluorfen), radio-labelled: 5-[2-chloro-4-(trifluoro-methyl)-phenoxy]-2-nitro benzoic acid-UL-14C, radiochemical purity 99.6% (HPLC) and 5-[2-chloro-4-(trifluoro-methyl)-phenoxy-UL-14C]-2-nitro benzoic acid, radiochemical purity 95.27% (HPLC)

Conclusion : t1/2 = 78-100 hrs

Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

26.12.2001 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	> 1 year at 25 degree C
t1/2 pH7	:	> 1 year at 25 degree C
t1/2 pH9	:	> 1 year at 25 degree C
Deg. Product	:	
Method	:	
Year	:	2001
GLP	:	no
Test substance	:	
Remark	:	Estimated on chemical principles based on absence of groups susceptible to hydrolysis The estimation program in EPIWIN has no capability to estimate hydrolysis rates for this compound.
Result	:	This material has no groups that are susceptible to hydrolysis in the pH 4 to 9 range; therefore, it is considered stable to hydrolysis in surface and groundwater. It is estimated to have a hydrolysis half-life of greater than one year between pH 4 and pH 9.
Test substance	:	Acifluorfen CAS 50594-66-6
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (6)

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air (level I)	:	
Water (level I)	:	
Soil (level I)	:	
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	
Year	:	2001
Method	:	The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Measured and estimated values were used for physical constants. Biodegradation was based on information in the EPA Reregistration Documentation and data in HSDB. The aquatic soil and

sediment estimates are estimates of an average half life from biodegradation and photolysis. As sediment distribution was low the half life estimate for water was used in the model. Half life in air was set at a default rapid loss since this material is not volatile. Emissions were calculated from using only water and soil as this test substance it is not volatile. Other parameters used the default values found in EPIWIN

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name   : Acifluorfen
  Molecular Wt: 361.66
  Henry's LC  : 6.03e-011 atm-m3/mole (Henrywin program)
  Vapor Press : 3.94e-008 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.54e-006 mm Hg  (super-cooled)
  Melting Pt  : 186 deg C (Mpbpwin program)
  Log Kow     : 3.7  (Kowwin program)
  Soil Koc    : 2.05e+003  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       4.41e-009       296          0
   Water     14.1            3.6e+003     1000
   Soil      83.8            3.6e+003     1000
   Sediment  2.09            1.44e+004    0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
Air       1.13e-019    6.22e-007   2.66e-006   3.11e-008   1.33e-007
Water     7.09e-016    164         853         8.21        42.7
Soil      9.45e-016    974         0           48.7        0
Sediment  1.05e-015    6.08        2.53        0.304       0.126

   Persistence Time: 3.02e+003 hr
   Reaction Time:    5.28e+003 hr
   Advection Time:   7.06e+003 hr
   Percent Reacted:  57.2
   Percent Advected: 42.8

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      296.4
      Water:    3600
      Soil:     3600
      Sediment: 1.44e+004
        Biowin estimate: 1.541  (recalcitrant)

   Advection Times (hr):
      Air:      100
      Water:    1000
       Sediment: 5e+004
```

g

Test substance : Acifluorfen CAS 50594-66-6
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (5)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum :
Remark : Studies are reported in the EPA RED documentation. This material

undergoes aquatic biodegradation with and estimated (EPA) half-life of 117 days.

Test substance : CAS 62476-59-9 (acifluorfen sodium)

Expected to biodegrade at essentially the same rate in the environment.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
27.12.2001 (4)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Anabaena flos-aquae (Algae)
Endpoint	:	other: biomass/growth rate
Exposure period	:	120 hour(s)
Unit	:	µg/l
Analytical monitoring	:	yes
NOEC	:	355
EC50	:	> 355
Method	:	other: EPA FIFRA 123-2
Year	:	1982
GLP	:	yes
Test substance	:	other TS
Method	:	TEST ORGANISMS - Species: Anabaena flos-aquae - Source/supplier: Carolina Biological Supply Company, Burlington, North Carolina - Method of cultivation: stock cultures were maintained under test conditions and transferred to fresh medium once or twice a week. The inoculum used in the tests was extracted from a 5 day old stock culture. - Initial cell concentration: 0.3E4 cells/mL STOCK AND TEST SOLUTION AND THEIR PREPARATION - Vehicle, solvent: none DILUTION WATER - Source: MBL medium GROWTH/TEST MEDIUM CHEMISTRY - Chemistry (P = 1.55 mg/L, N = 14 mg/L, Ca+Mg = 0.40 mmol/L, no EDTA) - pH 7.5 TEST SYSTEM - Test type: static - Concentrations: 370 ug a.i./L, control - Exposure vessel type: 125 mL flask containing 50 mL test solution (covered; shaken at 100 rpm) - Number of replicates: 3 - Photoperiod: continuous illuminated at 1700-2000 lux PHYSICAL MEASUREMENTS - Measuring times: 0 and 120 h - Test temperature: 25-26 C - pH: 7.4 at 0 hours, 9.2-9.4 at 120 hours DURATION OF TEST: 120 hours

TEST PARAMETER: cell counts by a haematocytometer
OBSERVATION TIMES: 24, 48, 72, 96 and 120 hours

ANALYSES
- Method: direct HPLC
- Sampling times: 0 and 120 hours

STATISTICAL METHOD: t-test, one-way analysis of variance, Dunnett's test, Chi-Square test, Hartley's test, Kruskal-Wallis test

Result : RESULTS:
- Nominal concentrations (ug a.i./L): 0, 370
- Meas. concentrations (ug a.i./L): 0, 355
- Cell density data: see attached document
- Inhibition-growth rate: 0, -11%
- Inhibition-biomass(AUC): 0, -3%

GROWTH FACTOR CONTROL: 100 after 72 hours

STATISTICAL RESULTS: no statistical differences in cell densities.

ANALYTICAL METHOD:
The analytical method was validated by fortifying water samples with 0.025, 0.25 and 3.0 mg/L. The recoveries of this samples (3x3) were 81-103%.

QCs (filtered (n=2) and unfiltered (n=2)) fortified at 25, 101, 202 ug a.i./L showed recoveries of respectively <LOQ-159%, 96-106%, 92-119%. For the 25 ug a.i./L the unfiltered samples showed recoveries of 159% (0 h) and 105% (120 h), the filtered samples showed recoveries of 67% (0 h) and <LOQ (120 h).

Source : Notox Hertogenbosch
Test substance : III, CAS 50594-66-6 (acifluorfen), purity 43,9%, impurities not specified
Attached doc. : BASF ref 80A.xls
Conclusion : 120 h EC50 >370 mg a.i./L (nominal)
120 h EC50 >355 mg a.i./L (measured)
Reliability : (1) valid without restriction
1. Anabaena is not one of the recommended test species of OECD 203, it is a recommendedn test species of the EPA. Light intensity was not in accordance with the guidelines (1700-2000 lux, OECD 201 8000 lux, EPA 2200 lux).
2. The medium used was not in accordance with OECD 201 (P: 1.55 mg/L, OECD 201 <=0.7 mg/L, N: 14 mg/L, OECD 201 <=10 mg/L). Higher P and N values may lead to stronger cell growth during the test.
2. Rises in pH of 2 units were probably associated with strong cell growth due to CO2 depletion from test media and do not invalidate the test, since in controls within 72 hours an adequate growth factor of 60 was determined.

09.05.2001 (2)

Species : Navicula pelliculosa (Algae)
Endpoint : other: biomass/growth rate
Exposure period : 120 hour(s)

Unit	:	µg/l
Analytical monitoring	:	yes
NOEC	:	345
EC50	:	> 345
Method	:	other: EPA FIFRA 123-2
Year	:	1982
GLP	:	yes
Test substance	:	other TS
Method	:	TEST ORGANISMS - Species: Navicula pelliculosa - Source/supplier: Carolina Biological Supply Company, Burlington, North Carolina - Method of cultivation: stock cultures were maintained under test conditions and transferred to fresh medium once or twice a week. The inoculum used in the tests was extracted from a 8 day old stock culture. - Initial cell concentration: 0.3E4 cells/mL STOCK AND TEST SOLUTION AND THEIR PREPARATION - Vehicle, solvent: none DILUTION WATER - Source: MBL medium GROWTH/TEST MEDIUM CHEMISTRY - Chemistry (P = 1.55 mg/L, N = 14 mg/L, Ca+Mg = 0.40 mmol/L, no EDTA) - pH 7.5 TEST SYSTEM - Test type: static - Concentrations: 370 ug a.i./L, control - Exposure vessel type: 125 mL flask containing 50 mL test solution (covered; shaken at 100 rpm) - Number of replicates: 3 - Photoperiod: continuous illuminated at 4000-5000 lux PHYSICAL MEASUREMENTS - Measuring times: 0 and 120 h - Test temperature: 25-26 C - pH: 7.4-8.2 DURATION OF TEST: 120 hours TEST PARAMETER: cell counts by a haematocytometer OBSERVATION TIMES: 24, 48, 72, 96 and 120 hours ANALYSES - Method: direct HPLC - Sampling times: 0 and 120 hours STATISTICAL METHOD: t-test, one-way analysis of variance, Dunnett's test, Chi-Square test, Hartley's test, Kruskal-Wallis test
Result	:	RESULTS: - Nominal concentrations (ug a.i./L): 0, 370 - Meas. concentrations (ug a.i./L): 0, 345 - Cell density data: see attached document

- Inhibition-growth rate: 0, -3%
- Inhibition-biomass(AUC): 0, -7%

GROWTH FACTOR CONTROL: 87 after 72 hours

STATISTICAL RESULTS: no statistical differences in cell densities.

ANALYTICAL METHOD:
The analytical method was validated by fortifying water samples with 0.025, 0.25 and 3.0 mg/L. The recoveries of this samples (3x3) were 81-103%.

QCs (filtered (n=2) and unfiltered (n=2)) fortified at 25, 101, 202 ug a.i./L showed recoveries of respectively <LOQ-159%, 96-106%, 92-119%. For the 25 ug a.i./L the unfiltered samples showed recoveries of 159% (0 h) and 105% (120 h), the filtered samples showed recoveries of 67% (0 h) and <LOQ (120 h).

Source : Notox Hertogenbosch
Test substance : III, CAS 50594-66-6 (acifluorfen), purity 43,9%, impurities not specified
Attached doc. : BASF ref 80B.xls
Conclusion : 120 h EC50 370 ug/L (nominal)
120 h EC50 345 ug/L (measured)
Reliability : (1) valid without restriction
1. Navicula pelliculosa is not one of the recommended test species of OECD 203, it is a recommended test species of the EPA. Light intensity was not in accordance with the OECD guideline (4000-5000 lux, OECD 201 8000 lux, EPA 4300 lux).
2. The medium used was not in accordance with OECD 201 (P: 1.55 mg/L, OECD 201 <=0.7 mg/L, N: 14 mg/L, OECD 201 <=10 mg/L). Higher P and N values may lead to stronger cell growth during the test.

09.05.2001 (2)

Species : Selenastrum capricornutum (Algae)
Endpoint : other: growth rate, biomass
Exposure period : 120 hour(s)
Unit : µg/l
Analytical monitoring : yes
NOEC : 260
EC50 : > 260
Method : other: EPA FIFRA 123-2
Year : 1982
GLP : yes
Test substance : other TS
Method : TEST ORGANISMS
- Species: Selenastrum capricornutum
- Source/supplier: Carolina Biological Supply Company, Burlington, North Carolina
- Method of cultivation: stock cultures were maintained under test consitions and transferred to fresh medium once or twice a week. The inoculum used in the tests was extracted from a 7 day old stock culture.
- Initial cell concentration: 0.3E4 cells/mL

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none

DILUTION WATER
- Source: MBL medium

GROWTH/TEST MEDIUM CHEMISTRY
- Chemistry (P = 1.55 mg/L, N = 14 mg/L, Ca+Mg = 0.40 mmol/L, no EDTA)
- pH 7.5
TEST SYSTEM
- Test type: static
- Concentrations: 24, 47, 93, 185, 370 ug a.i./L, control
- Exposure vessel type: 125 mL flask containing 50 mL test solution (covered; shaken at 100 rpm)
- Number of replicates: 3
- Photoperiod: continuous illuminated at 4000-5000 lux
PHYSICAL MEASUREMENTS
- Measuring times: 0 and 120 h
- Test temperature: 25-26 C
- pH: 7.4 at 0 hours, 9.7-10.4 at 120 hours

DURATION OF TEST: 120 hours

TEST PARAMETER: cell counts by a haematocytometer
OBSERVATION TIMES: 24, 48, 72, 96 and 120 hours

ANALYSES
- Method: direct HPLC
- Sampling times: 0 and 120 hours

STATISTICAL METHOD: t-test, one-way analysis of variance, Dunnett's test, Chi-Square test, Hartley's test, Kruskal-Wallis test

Result : RESULTS:
- Nominal concentrations (ug a.i./L): 0, 24, 47, 93, 185, 370
- Meas. concentrations (ug a.i./L): 0, 19, 38, 88, 160, 260
- Cell density data: see attached document
- Inhibition-growth rate [%]: 0, -2, 0, 0, 0, 0
- Inhibition-biomass(AUC) [%]: 0, -12, -3, -3, -1, 0

GROWTH FACTOR CONTROL: 144 after 72 hours

STATISTICAL RESULTS: no statistical differences in cell densities.

ANALYTICAL METHOD:
The analytical method was validated by fortifying water samples with 0.025, 0.25 and 3.0 mg/L. The recoveries of this samples (3x3) were 81-103%.

QCs (filtered (n=2) and unfiltered (n=2)) fortified at 25, 101, 202 ug a.i./L showed recoveries of respectively <LOQ-159%, 96-106%, 92-119%. For the 25 ug a.i./L the unfiltered samples showed recoveries of 159% (0 h) and 105% (120 h), the filtered samples showed recoveries of 67% (0 h)

and <LOQ (120 h).

Source : Notox Hertogenbosch
Test substance : III, CAS 50594-66-6 (acifluorfen), purity 43,9%, impurities not specified
Attached doc. : BASF ref 80.xls
Conclusion : 120 h EC50 >370 mg a.i./L (nominal)
120 h EC50 >260 mg a.i./L (measured)
Reliability : (1) valid without restriction
1. The medium used was not in accordance with OECD 201 (P: 1.55 mg/L, OECD 201 <=0.7 mg/L, N: 14 mg/L, OECD 201 <=10 mg/L). Higher P and N values may lead to stronger cell growth during the test. Light intensity was lower than recommended (4000-5000 lux, OECD 201 8000 lux), which could decrease the cell growth.
2. Rises in pH of 2-3 units were probably associated with strong cell growth due to CO2 depletion from test media and do not invalidate the test, since in controls within 72 hours an adequate growth factor of 144 was determined.

09.05.2001 (2)

Species : Skeletonema costatum (Algae)
Endpoint : other: biomass/growth rate
Exposure period : 120 hour(s)
Unit : µg/l
Analytical monitoring : yes
NOEC : 300
EC50 : > 300
Method : other: EPA FIFRA 123-2
Year : 1982
GLP : yes
Test substance : other TS
Method : TEST ORGANISMS
- Species: Skeletonema costatum
- Source/supplier: Bigelow marine Laboratory, West Boothbay, Maine
- Method of cultivation: stock cultures were maintained under test conditions and transferred to fresh medium once or twice a week. The inoculum used in the tests was extracted from a 9 day old stock culture.
- Initial cell concentration: 1.0E4 cells/mL

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none

DILUTION WATER
- Source: Artificially Enriched Seawater prepared with filtered natural seawater

GROWTH/TEST MEDIUM CHEMISTRY
- Chemistry (P = 0.44 mg/L, N = 8.2 mg/L, no EDTA, salinity not indicated)
- pH 8.0

TEST SYSTEM
- Test type: static
- Concentrations: 370 ug a.i./L, control
- Exposure vessel type: 125 mL flask containing 50 mL test

solution (covered; shaken at 60 rpm)
- Number of replicates: 3
- Photoperiod: 16 hours light (4000-5000 lux)
PHYSICAL MEASUREMENTS
- Measuring times: 0 and 120 h
- Test temperature: 20-23 C
- pH: 8.2-8.9

DURATION OF TEST: 120 hours

TEST PARAMETER: cell counts by a haematocytometer
OBSERVATION TIMES: 24, 48, 72, 96 and 120 hours

ANALYSES
- Method: direct HPLC
- Sampling times: 0 and 120 hours

STATISTICAL METHOD: t-test, one-way analysis of variance, Dunnett's test, Chi-Square test, Hartley's test, Kruskal-Wallis test

Result : RESULTS:
- Nominal concentrations (ug a.i./L): 0, 370
- Meas. concentrations (ug a.i./L): 0, 300
- Cell density data: see attached document
- Inhibition-growth rate: 0, 0%
- Inhibition-biomass(AUC): 0, 1%

GROWTH FACTOR CONTROL: 59 after 72 hours

STATISTICAL RESULTS: no statistical differences in cell densities.

ANALYTICAL METHOD:
The analytical method was validated by fortifying water samples with 0 and 379 ug/L. The recoveries of this samples (n=3) were 100-101%.

QCs (n=2x2) fortified at 101, 202 and 303 mg a.i./L showed recoveries of 96-107% (filtered) and 69-84% (unfiltered).

Source : Notox Hertogenbosch

Test substance : III, CAS 50594-66-6 (acifluorfen), purity 43,9%, impurities not specified

Attached doc. : BASF ref 80C.xls

Conclusion : 120 h EC50 370 ug/L (nominal)
120 h EC50 300 ug/L (measured)

Reliability : (1) valid without restriction
1. Skeletonema costatum is not one of the recommended test species of OECD 203, but a marine diatom recommended by the EPA. Light intensity was not in accordance with the OECD guideline (4000-5000 lux, OECD 201 8000 lux, EPA 4300 lux).
2. Salinity was not indicated, but since natural seawater was used for the preparation of the test medium, the reliability was not lowered.
3. The QCs were reported to be fortified at 101-303 mg a.i./L. Probably this is a reporting error and the actual fortification was 101-303 ug a.i./L.

09.05.2001 (2)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	TA98, TA100, TA1535 and TA1537
Concentration	:	20-5000 ug/plate
Cycotoxic conc.	:	5000 ug/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year	:	
GLP	:	
Test substance	:	other TS
Method	:	SYSTEM OF TESTING: - Species/cell type: Salmonella typhimurium TA98, TA100, TA1535, TA1537. - Deficiences/Proficiences: histidine - Metabolic activation system: rat S9 mix (Arochlor 1254 induced) ADMINISTRATION: - Dosing: 0, 20, 100, 500, 2500 and 5000 µg/plate: - Number of replicates: 3 - Application: DMSO - Positive and negative control groups and treatment: Positive controls:

Without S-9: 2-N-methyl-N'-nitroso-guanidine (MNNG) (TA100 and TA1535); 4-nitro-o-phenylenediamine (TA98); 9-aminoacridine chloride monohydrate (TA1537)
With S-9: 2-aminoantharacene
Negative controls: DMSO
- type of test: direct plate assay

CRITERIA FOR EVALUATING RESULTS: number of revertant colonies

Result : No precipitation was observed.

Slight toxicity to strains TA1535 and TA100 at 5000 ug/plate.

Source : Notox Hertogenbosch

Test substance : CAS 50594-66-6, (5-(2-chloro-4-trifluoromethylphenoxy) -2-nitrobenzoic acid), purity 99.5%

Reliability : (2) valid with restrictions
1.Test results for the purity and stability of the compound are not included in the report.
2. Only 4 strains of bacteria are used (OECD 471: at least 5 strains)
3. 2-aminoanthracene alone as positive control is not sufficient according to OECD guideline 471. However, as the positive control induced a sufficient number of revertant colonies, reliability is not lowered.
4. No GLP

16.05.2001 (1)

5.6 GENETIC TOXICITY 'IN VITRO'

5.7 CARCINOGENITY

5.8 TOXICITY TO REPRODUCTION

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Source : Notox Hertogenbosch
02.04.2001

5.10 OTHER RELEVANT INFORMATION

5.11 EXPERIENCE WITH HUMAN EXPOSURE

(1) BASF Aktiengesellschaft, Report on the study of Acifluoren-Reinwirkstoff in the Ames Test, 1990

(2) BASF, Acifluorfen (BAS 9048 H): toxicity to the growth and reproduction of aquatic plants, 1990 (80)

(3) BASF, Artificial Sunlight Photolysis of Acifluorfen in Aqueous Media at pH 7.0 (1993) (87).

(4) EFED Ecological Risk Assessment for sodium acifluorfen. US EPA, Registration Process Documents, June 2000. http://www.epa.gov/pesticides/reregistration/acifluorfen/efedchapter.pdf

(5) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(6) Lyman, W. J. et al. (1990). Handbook of Chemical PropertyEstimation Methods, pp. 7-4, Amer. Chem. Society,Washington, DC

(7) SRC PHYSPROP Database. http://esc.syrres.com/interkow/physdemo.htm

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

I U C L I D

Data Set

Existing Chemical	:	ID: 62476-59-9
CAS No.	:	62476-59-9
Generic name	:	Sodium 5-(2-chloro-4-trifluoro-methylphenoxy) 2-nitrobenzoate

Producer related part

Company	:	BASF Corporation
Creation date	:	19.02.2003

Substance related part

Company	:	BASF Corporation
Creation date	:	19.02.2003
Status	:	
Memo	:	
Printing date	:	21.02.2003
Revision date	:	
Date of last update	:	19.02.2003
Number of pages	:	204
Chapter (profile)	:	Chapter: 2.1, 2.2, 2.4, 2.5, 2.6.1, 3.1.1, 3.1.2, 3.3.1, 3.5, 4.1, 4.2, 4.3, 5.1.1, 5.1.2, 5.1.3, 5.1.4, 5.4, 5.5, 5.6, 5.8.1, 5.8.2
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value : 172 °C
Decomposition : yes, at ca. 240 °C
Sublimation :
Method : OECD Guide-line 102 "Melting Point/Melting Range"
Year : 1981
GLP : no
Test substance : other TS

Method : capillary method/metal block apparatus
Result :

	determination 1	determination 2
beginning of melting (shrink point) (deg C)	172	172
collapse point (deg C)	178	178

No other melt transitions were noted. Samples were heated to 240 deg C when sample degradation was noted by disc
Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ
Test condition : Duplicate dried powder samples were charged into a capillary column (resulting height about 2 mm). Samples were initially heated in the melting point apparatus at about 5 deg C/min, and at about 1 deg C/min within 10 deg C of the transition. Method was validated using a reference substance of known melting point (sulfanilamide).
Test substance : III, CAS 62476-59-9 (acifluorfen-sodium, purified technical), purity 89.3%
Conclusion : Melting starts at 172 deg C. Melting is not complete; test substance decomposes at about 240 deg C.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
26.12.2001 (18)

Value : 176 °C
Decomposition : yes, at ca. 240 °C
Sublimation :
Method : OECD Guide-line 102 "Melting Point/Melting Range"
Year : 1981
GLP : no
Test substance : other TS

Method : capillary method/metal block apparatus
Result :

	determination 1	determination 2
beginning of melting (shrink point) (deg C)	176	176

No other melt transitions were noted. Samples were heated to 240 deg C when sample degradation was noted by di
Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ
Test condition : Duplicate dried powder samples were charged into a capillary column (resulting height about 2 mm). Samples were initially heated in the melting point apparatus at about 5 deg C/min, and at about 1 deg C/min within 10 deg C of the transition. Method was validated using a reference substance of known

melting point (sulfanilamide).

Test substance	:	III, CAS 62476-59-9 (acifluorfen-sodium, technical), purity 74.4%
Conclusion	:	Melting starts at 176 deg C. Melting is not complete; test substance decomposes at about 240 deg C.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

26.12.2001 (18)

2.2 BOILING POINT

2.4 VAPOUR PRESSURE

Value	:	< .000000133 hPa at 25 °C
Decomposition	:	no
Method	:	other (measured): essentially OECD 104 (gas saturation method)
Year	:	1981
GLP	:	yes
Test substance	:	other TS
Result	:	In all cases, acifluorfen sodium could either not be detected or its vapor pressure was < 1.33E-5 Pa, which is the lower limit of detection.
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test condition	:	Vapor pressure was measured at 25, 35 and 45 +/- 0.5 deg C using 8 or 9 flow rates in the range 7-140 cc/min. At 25 and 45 deg C two experiments were performed. Hereto, acifluorfen sodium was packed into 5 mm glass tubing between 2 glass wool plugs (sample length 60 mm) and connected to 2 XAD-2 sorbent sections separated by glass wool (about 15 and 10 mm). The system was placed in a constant temperature box and nitrogen gas was passed through it. After at least 473 hrs, the sorbent traps were extracted with 2 mL methanol and 1 mL water (shaking for 2 hrs). The extracts were analyzed by HPLC; quantitation was performed using standard solutions of acifluorfen sodium (prepared from acifluorfen) in methanol in the range 0.5-5.0 ug/mL. Blank sample tubes were included for each temperature.
Test substance	:	III, CAS 62476-59-9 (acifluorfen sodium), purity 89.3%
Conclusion		VP < 1.33E-5 Pa
Reliability	:	(2) valid with restrictions 1. For all blank sample tubes TS appeared to be recovered (or a contaminant with an identical retention time). Therefore, the experiment was repeated at 25 and 45 deg C with 5 blanks (3 tubes containing glass wool, 2 empty glass tubes), but blanks contained TS again (or contaminant). In only one of the 39 sample tubes did the compound detected exceed the apparent concentrations found in the blanks.
Flag	:	Critical study for SIDS endpoint

26.12.2001 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	at 25 °C
pH value	:	

Method : other (measured): essentially OECD 107
Year : 1995
GLP : yes
Test substance : other TS

Method : Test solutions of acifluorfen sodium in octanol/aqueous buffer at a ratio of approximately 1:1 (v/v) (pH 5, 7 and 9) were prepared. Hereto, equimolar amounts of acifluorfen acid (CAS 50594-66-6, purity 99.4%, dissolved in buffer-saturated octanol) and sodium hydroxide (dissolved in octanol-saturated buffer) were mixed, followed by the addition of octanol. Triplicate samples of two concentration levels (appr. 8 mM and 0.8 mM in the original octanol phase) were prepared for each pH. Total volume was 0.02 L, except for pH 7, high concentration level (total volume 0.05 L). The samples were shaken at 25 +/- 1 deg C for 16 hours, centrifugated, and each octanol and water phase was diluted with mobile phase and analyzed by liquid chromatography using acifluorfen acid (purity 99.5%) as a reference standard.

Result : Buffer pH Initial TS concentration in n-octanol (mM) Kow (mean of 3 replicates)

5	8	15.6 +/- 0.17
7	8	1.88 +/- 0.04
9	8	1.46 +/- 0.05
5	0.8	15.6 +/- 0.81
7	0.8	1.21 +/- 0.06
9	0.8	1.12 +/- 0.03

At pH 5 there is no concentration dependence of Kow.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (acifluorfen sodium), purity 99.4% as acid prior to conversion to sodium salt.

Conclusion :

	Kow*	log Kow*
pH 5	15.6	1.19
pH 7	< 2	< 0.3
pH 9	< 1.5	< 0.2

*(mean of two conce

Reliability : (2) valid with restrictions
Remarks:
1. TS is in the ionized form, which may cause deviations from the partition law. Method is not suitable for ionized substances. OECD 107 advises adjustment of pH to 1 unit below or above the pK, but in this case this is not applicable as TS is a salt and should therefore not be protonated.

2. Test was performed at only one water:octanol ratio for each pH and TS concentration.

Flag : Critical study for SIDS endpoint
26.12.2001 (6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : 405 other: mg/g at 25 °C

pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	moderately soluble (100-1000 mg/L)
Stable	:	
Deg. product	:	
Method	:	other: essentially OECD 105
Year	:	1981
GLP	:	yes
Test substance	:	other TS

Method : Six centrifuge tubes with test mixture (approximately 10 g TS/10 mL in HPLC grade water) and two blanks (to check for interference in the analysis) were shaken in a water bath of 35 +/- 1 deg C for about 4 hrs, followed by transfer to a 25 +/- 1 deg C water bath (continueous shaking). After 3, 6 and 7 days aliquots were removed after centrifugation at appr. 31,300 x G or 41,300 x G (3 replicates and 1 blank each) for 30 min. at 25 +/- 1 deg C. About 0.5 mL was weighed, diluted by a factor 1000 and analyzed by LC (duplicate injection). Standard solutions in the range 0.370-0.685 mg/mL were included for quantification, as well as a reference acifluorfen acid control solution to check recovery.

Result : Day Acifluorfen sodium (mg/g) at centrifuge speed:

Day	31,300xG*	41,300xG*	Mean
3	411.6	405.7	409 +/- 6
6	404.3	407.4	406 +/- 5
7	396.0	407.2	402 +/- 8

* mean of three replicates, calculated by reviewer to summarize data

Overall mean: 405 +/- 6.3 mg/g
Statistical analysis indicated no statistically significant difference between days 3, 6 and 7. Hence, equilibrium had been established.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (acifluorfen sodium), purity 78.2%

Conclusion : Water solubility of acifluorfen sodium = 405 +/- 6.3 mg/g.

Reliability : (1) valid without restriction
minor remark:
1. Purity of the test substance was only 78.2%. Impurities may influence the solubility of acifluorfen sodium. No information on the identity of the remainder of the test substance was given.

Flag : Critical study for SIDS endpoint
14.05.2001 (5)

3.1.1 PHOTODEGRADATION

Type	:	water
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Remark	:	Indirect photolysis is not considered as this material is not volatile. Several studies are reported in the EPA RED documentation. It is apparent that this material undergoes primary photodegradation; however, the exact rate and spectrum of degradation products is not fully understood.
Result	:	Half life values ranged from 21 hours to 352 hours depending on concentrations and conditions. Near neutrality a mid estimate is 90 hours.
Source	:	Toxicology and Regulatory Affairs Flemington NJ
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

26.12.2001 (9)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Degradation	:	0 % after 28 day(s) at pH and °C
Deg. product	:	
Method	:	other: essentially OECD 111
Year	:	1981
GLP	:	no
Test substance	:	other TS
Method	:	Test solutions (1.0 ppm and 50.0 ppm TS; buffered to pH 4.5, 7.2 and 9.7) were incubated at 25 deg C in complete darkness for 28 (1.0 ppm samples) and 56 days (50.0 ppm samples). No cosolvent was used. Samples were taken on day 0,1,3,7,14 and 28 (1.0 ppm samples) and on day 0,1,3,7,14,28 and 56 (50 ppm samples). 0.1 N H3PO4 was added to samples (conversion of sodium acifluorfen to free acid) followed by extraction with benzene. Both aqeous and benzene fractions were analyzed by LSC, benzene fractions were also subjected to TLC.
Result	:	Day Nominal concentration sodium acifluorfen

Day	(ppm)	(ppm) pH 4.5	pH 7.2	pH 9.7
0	50	46.82*	48.87	49.12
7	50	50.77	49.61	49.19
14	50	57.61	55.87	53.03
28	50	50.90	50.63	49.18
56	50	53.45	53.14	51.43
0	1	1.04	1.06*	1.06
7	1	1.11	1.14	1.12
14	1	1.26	1.26	1.27

28 1 1.09 1.12 1.12

Mass balances were in the range 84.5-98.7% at all time points, except at for samples and time points marked with *. For these, mass balances were < 17%, which is explained by low extraction efficiencies. Extraction efficiency was improved by addition of 1 mL 0.1 N H3PO4 before extraction with benzene from day 7 onwards.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (sodium acifluorfen), radio-labelled, purity 99%, specific activity 4706 dpm/ug

Conclusion : Test substance is stable in water.

Reliability : (2) valid with restrictions
1. Volatiles were not measured (no traps), which is said to be of no concern because of high mass balance. In addition, an increase with time of TS concentration was observed, which is explained by evaporation of solvent. TLC results are only quantified for day 7 (no reference standard). An exact mass balance can therefore not be calculated.
2. The report consisted of a summary rather than a full report. In this summary, only testing at 25 deg C is described, whereas results for 2 other temperatures (36 and 48 deg C) are also given. Results for the other 2 temperatures support the conclusion of the test at 25 deg C.
3. Sterility was not measured, nor was the sterility of the buffers included in the study. However, as hardly any degradation was observed, biotic degradation can be excluded.

Flag : Critical study for SIDS endpoint

10.05.2001 (7)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air :
Water :
Soil :
Biota :
Soil :
Method :
Year : 2001

Method : The Fugacity was determined using the EQC Level III model as found in EPIWIN 3.05. Measured values were used for most physical constants. Biodegradation was based on information in the EPA Reregistration Documentation and data in HSDB. The aquatic soil and sediment estimates are estimates of an average half life from biodegradation and photolysis. As sediment distribution was low the half life estimate for water was used in the model. Half life in air was set at a default rapid loss since this material is not volatile. Emissions were calculated from using only water and soil as this test substance it is not volatile. Other parameters used the default values found in EPIWIN.

Result :

```
Level III Fugacity Model (Full-Output):
=======================================
  Chem Name    : Sodium Acifluorfen
```

```
Molecular Wt: 383.65
Henry's LC  : 1.25e-012 atm-m3/mole (calc VP/Wsol)
Vapor Press : 1e-007 mm Hg  (user-entered)
Liquid VP   : 2.84e-006 mm Hg  (super-cooled)
Melting Pt  : 172 deg C (user-entered)
Log Kow     : 0.37  (Kowwin program)
Soil Koc    : 0.961  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
Air       1.05e-010       24          0
Water     60.4            1.44e+003   1000
Soil      39.5            960         1000
Sediment  0.103           1.44e+003   0

         Fugacity    Reaction    Advection   Reaction    Advection
          (atm)       (kg/hr)      (kg/hr)    (percent)   (percent)
Air       8.62e-022    5.14e-008   1.78e-008   2.57e-009   8.91e-010
Water     1.66e-017    493         1.02e+003   24.6        51.2
Soil      3.74e-016    483         0           24.1        0
Sediment  1.38e-017    0.838       0.0348      0.0419      0.00174

   Persistence Time: 847 hr
   Reaction Time:    1.74e+003 hr
   Advection Time:   1.65e+003 hr
   Percent Reacted:  48.8
   Percent Advected: 51.2

   Half-Lives (hr), (based upon user-entry):
      Air:      24
      Water:    1440
      Soil:     960
      Sediment: 1440

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

Source : Toxicology and Regulatory Affairs Flemington NJ
Test substance : CAS 62476-59-9 (acifluorfen sodium)
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (10)

3.5 BIODEGRADATION

Type : aerobic
Inoculum :

Remark : Studies are reported in the EPA RED documentation. This material undergoes aquatic biodegradation with and estimated (EPA) half-life of 117 days.
Source : Toxicology and Regulatory Affairs Flemington NJ
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
26.12.2001 (8)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Lepomis macrochirus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	62
Limit test	:	
Analytical monitoring	:	yes
Method	:	other: EPA 660/3-75-009
Year	:	1975
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS
- Species: Lepomis macrochirus
- Supplier: Commercial fish supplier in Missouri
- Size;weight;loading: 30-38 mm; 0.31-0.73 g; <0.5 g/L
- Feeding (pretreatment): dry pelleted food daily, ad libitum; discontinued 48 hours prior to test initiation
- Feeding during test: none

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none

DILUTION WATER
- Source: deionized, reconstituted water
- Chemistry (Alkalinity 32-34 mg/L;Hardness 42 mg CaCO3/L;pH 7.4;Conductance 130-160 umhos/cm)

TEST SYSTEM
- Test type: static
- Concentrations: 0, 22, 36, 60, 100 and 170 mg a.i./L
- Exposure vessel type: 20 L glass jars containing 15 L of test water
- Number of fish: 10 per treatment
- Photoperiod: 16 hours

PHYSICAL MEASUREMENTS
- Measuring times: 0, 24, 48, 72, 96 hours
- Test temperature: 22-23 C
- Dissolved oxygen: 73-100% (0-24 h), 52-68% (48 h), 45-73% (72 h), 40-77% (96 h)
- pH: 6.6-7.3

DURATION OF THE TEST: 96 hours

TEST PARAMETER: mortality/symptoms
OBSERVATION TIMES: 24, 48, 72, 96 hours

ANALYSES
- Method: not specified
- Sampling times: 0, 96 hours

STATISTICAL METHOD: moving average angle analysis

Result : RESULTS:
- Nominal concentrations (mg a.i./L): 0, 22, 36, 60, 100, 170
- Mortality [%]: 0, 0, 10, 20, 100, 100
- Other effects: fish at surface, dark discoloured,

respiring rapidly and /or swimming erratically at 60 and 100 mg a.i./L
- Effect concentration vs. test substance solubility: At 100 and 170 mg a.i./L the test solution had a cloudy appearance, which could indicate undissolved substance

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (Sodium acifluorfen), purity 25% (impurities not specified)

Conclusion : 96 h LC50 62 mg a.i./L (95% CI 49-80 mg a.i./L)

Reliability : (2) valid with restrictions
1. No analytical results were presented in this report. It cannot be excluded that the actual concentration differed from the nominal, at least at the highest test concentrations (cloudy appearance indicating undissolved substance). The study reliability is lowered because of this.
2. Fish may have been more sensitive due to the low oxygen concentration during the test (40-100%, OECD 203 >60%) and the long fasting (48 hours, OECD 203 24 hours).
3. The used fish were larger than recommended by OECD 203, but acceptable according to the EG-guideline (30-38 mm, OECD 202 20+/-10 mm, EG 50+/-20 mm).

09.05.2001 (15)

Type : static
Species : Salmo gairdneri (Fish, estuary, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : 17
Limit test :
Analytical monitoring : yes
Method : other: EPA 660/3-75-009
Year : 1975
GLP : no
Test substance : other TS

Method : TEST ORGANISMS
- Species: Salmo gairdneri
- Supplier: Commercial fish supplier in Nebraska
- Size;weight;loading: 30-45 mm; 0.18-0.67 g; 0.3 g/L
- Feeding (pretreatment): dry pelleted food daily, ad libitum; discontinued 48 hours prior to test initiation
- Feeding during test: none

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Vehicle, solvent: none

DILUTION WATER
- Source: deionized, reconstituted well water
- Chemistry (Alkalinity 32 mg/L;Hardness 40 mg CaCO3/L;pH 7.2;Conductance 110 umhos/cm)

TEST SYSTEM
- Test type: static
- Concentrations: 0, 4.6, 7.8, 13, 22 and 36 mg a.i./L
- Exposure vessel type: 20 L glass jars containing 15 L of test water
- Number of fish: 10 per treatment
- Photoperiod: 16 hours

PHYSICAL MEASUREMENTS
- Measuring times: 0, 24, 48, 72, 96 hours

- Test temperature: 12 C
- Dissolved oxygen: 69-99% (0-72 h), 50-64% (96 h)
- pH: 6.8-7.2

DURATION OF THE TEST: 96 hours

TEST PARAMETER: mortality/symptoms
OBSERVATION TIMES: 24, 48, 72, 96 hours

ANALYSES
- Method: not specified
- Sampling times: 0, 96 hours

STATISTICAL METHOD: binomial probability

Result : RESULTS:
- Nominal concentrations (mg a.i./L): 0, 4.6, 7.8, 13, 22, 36
- Measured concentrations (mg/L): not reported
- Mortality [%]: 0, 0, 0, 0, 90, 100
- Other effects: swimming erratically, dark coloured, staying at the surface and/or lethargic at 13-36 mg a.i./L

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (Sodium acifluorfen), purity 25% (impurities not specified)

Conclusion : 96-h LC50 17 mg a.i./L (95% CI 13-22 mg a.i./L)
96-h NOEC 7.8 mg a.i./L

Reliability : (2) valid with restrictions
1. No analytical results were presented in this report, so it cannot be excluded that the actual concentration differed from the nominal. The study reliability is lowered because of this.
2. Fish may have been more sensitive due to the long fasting (48 hours, OECD 203 24 hours) and due to their small size (30-45 mm, OECD 203 50+/-10 mm).

09.05.2001 (14)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : 77
Analytical monitoring : yes
Method :
Year :
GLP : no
Test substance : other TS

Method : TEST ORGANISMS
- Species: Daphnia magna
- Source/supplier: Bionomics culture facility
- Breeding method: Culture of Daphnia in water with hardness of 165 mg CaCO3/L, pH 7.9-8.3, temperature 22+/-1 C, Oxygen >60% (same as test water)
- Age: <= 20 hours
- Feeding before and during test: not specified

STOCK AND TEST SOLUTION AND THEIR PREPARATION

- Vehicle, solvent: none

DILUTION WATER
- Source: Deionized, reconstituted well water
- Chemistry (Alkalinity 120 mg/L;Hardness 160-170 mg/L/pH 8.0-8.2/Conductance 440-450 umhos/cm)

TEST SYSTEM
- Test type: static
- Concentrations: 0, 13, 22, 36, 60, 100 mg a.i./L
- Exposure vessel type: 250 mL beakers containing 200 mL test solution
- Number of individuals: 5 per replicate, 4 replicates/treatment
- Photoperiod (intensity of irradiation): illuminated at 538-753 lux

PHYSICAL MEASUREMENTS
- Measuring times: 0, 24 (only temperature) and 48 hours
- Test temperature: 21 C
- Dissolved oxygen: 94-100%
- pH: 8.0-8.2

DURATION OF THE TEST: 48 hours

TEST PARAMETER: mortality/symptoms
OBSERVATION TIMES: 0, 24, 48 hours

ANALYSES
- Method: not specified
- Sampling times: 0 and 48 hours

STATISTICAL METHOD: moving average angle method

Result : RESULTS:
- Nominal concentrations (mg a.i./L): 0, 13, 22, 36, 60, 100
- Measured concentrations (mg/L): not reported
- Immobility [%]: 0, 0, 0, 13, 13, 90
- Other effects: lethargic at 36-100 mg/L

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (Sodium acifluorfen), purity 25% (impurities not specified)

Conclusion : 48 h EC50: 77 mg a.i./L (95% CI 66-94 mg a.i./L)

Reliability : (1) valid without restriction
1. Analyses were performed, but the results were not included in the report. Since analyses were not recommended by OECD 202, the study reliability was not lowered.
2. There was no information on the feeding of the Daphnia.

09.05.2001 (16)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 122 mg/kg bw
Species	:	rat
Strain	:	other: CF Nelson
Sex	:	male
Number of animals	:	10
Vehicle	:	water
Doses	:	
Method	:	other: not indicated
Year	:	
GLP	:	no
Test substance	:	other TS
Method	:	TEST ORGANISMS: - Source: not indicated - Age: not indicated - Number: 10/dose - Weight at study initiation: 196-201 g (mean) - Controls: no ADMINISTRATION: - Doses: 625, 1250, 2500 and 5000 mg/kg - Doses per time period: single - Volume administered or concentration: 20% (w/v) - Post dose observation period: 14 days - food withheld for 24 hours pre-dosing EXAMINATIONS: signs of intoxication and gross necropsy BODY WEIGHT: pre-dosing and at the end of the test STATISTICAL METHOD: not indicated
Result	:	MORTALITY: - Number of deaths at each dose: 625, 1250, 2500 and 5000 mg/kg bw: 0/10, 3/10, 9/10 and 10/10, resp. - Time of death: for the highest dose: within 6 hours, for the other doses: within two days. CLINICAL SIGNS: lethargy, prostration and ataxia at 2500 and 5000 mg/kg bw BODY WEIGHT: no effects NECROPSY FINDINGS: no visible lesions in the survivors
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	III, CAS 62476-59-9 (sodium 5-(2-chloro-4-trifluoro-methylphenoxy)2-nitrobenzoate, purity 39.6%, used as 20% (w/v) aqueous dispersion
Conclusion	:	LD50 1540 mg/kg bw
Reliability	:	(2) valid with restrictions 1. The information was essentially confined to what is included in the current summary. No individual data were present.

04.01.2002 (21)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	> 1.38 mg/l
Species	:	rat
Strain	:	other: albino King (Kng:(SD)BR)
Sex	:	male/female
Number of animals	:	10
Vehicle	:	other: no vehicle
Doses	:	
Exposure time	:	4 hour(s)
Method	:	other: not indicated
Year	:	
GLP	:	no
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Source: King Animal Laboratories, Inc., Oregon, WI
- Age: not specified
- Weight at study initiation: males (246-291 g) and females (217-248 g)
- Number of animals: 5/sex/dose
- Controls: yes

ADMINISTRATION:
- Type of exposure: whole body exposure to aerosol
- Exposure duration: 4 hours
- Concentrations(nominal/measured): 17.9 / 6.91 mg/l (analytical conc.) or 2.6 mg/l (gravimetric conc.)
- Particle size: mass median diameter: 2.11 micrometer with standard deviation 2.59 micrometer (first sample) and 3.65 micrometer with standard deviation of 2.20 micrometer (second sample).
- Type or preparation of particles: air atomizing nozzle assembly
- Air changes: >= 15/hr

EXAMINATIONS: for pharmacotoxic signs (during exposure and twice daily during 14 days post-exposure time); gross necropsy

BODY WEIGHT: pre-exposure and at days 7 and 14

ANALYSES:
- Method: gravimetry and analytical concentration by extraction/spectrophotometry
- Sampling times: 4 times/4 hours
- Particle size determination at 1 and 3 hours

STATISTICAL METHOD: not specified

Result :

MORTALITY:
- Number of deaths at each dose: no deaths

CLINICAL SIGNS: during exposure: squinting, nasal discharge, dyspnea and lacrimation; shortly after exposure: nasal discharge, dyspnea, crusty nose and yellow/brown stained fur; during the 14-day observation period: nasal discharge, crusty nose, yellow/brown stained fur, crusty mouth and poor coat quality.
The control group did not show any clinical signs

BODY WEIGHT: no treatment-related effects

NECROPSY FINDINGS: one treated rat with focal depressions of the lung; for the control animals: 2 rats with lung lesions and 1 rat with diaphramatic hernia of the liver.

SEX-SPECIFIC DIFFERENCES: no data

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (TACKLE 2AS formulation), 20% w/w aqueous solution

Conclusion : LC50 > 6910 mg/m3

Reliability : (2) valid with restrictions
1. The obtainment of the results for the exposure chamber (nominal concentration, airchanges/hr) are unclear.
2. The gravimetric measured concentration of 2.6 mg/l is less reliable than the analytical measured concentration.
3. Only a QA statement was included, but no GLP statement signed by the study director.

04.01.2002 (22)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : = 1457 mg/kg bw
Species : rabbit
Strain : other: Albino
Sex : male
Number of animals : 5
Vehicle : other: no vehicle
Doses :
Method : other: not specified
Year :
GLP : no
Test substance : other TS

Method : TEST ORGANISMS:
- Source: not indicated
- Age: not indicated
- Weight at study initiation: 2.71-2.86 kg (mean)
- Controls: no

ADMINISTRATION:
- Area covered: not specified
- Occlusion: yes
- Vehicle: no vehicle, test substance is an aqueous solution
- Doses: 2500, 3540 and 5000 mg/kg bw
- Removal of test substance: not indicated

EXAMINATIONS: signs of intoxication, skin irritation and gross necropsy

BODY WEIGHT: pre-dosing and at end of the test

STATISTICAL METHOD: not indicated

Result : MORTALITY:
- Number of deaths at each dose: 2500, 3540 and 5000 mg/kg bw: 1/5, 2/5 and 4/5, resp.
- Time of death: at 2500 and 3540 mg/kg bw, within 4 days;

at 2500 mg/kg bw, between days 8 and 14.

CLINICAL SIGNS: lethargy, ataxia, shallow respiration and prostration; well defined to moderate erythema, slight edema, followed by desiccation and flaking of skin at 3540 and 5000 mg/kg bw.

BODY WEIGHT: increased bw for the lowest dose survivors; decreased bw for the two highest doses survivors.

NECROPSY FINDINGS: no visible lesions for the decendents at 3540 and 2500 mg/kg bw; no visible lesions for the survivors.

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (sodium 5-(2-chloro-4-trifluoro-methylphenoxy)2-nitrobenzoate, purity 39.6% aqueous technical

Conclusion : LD50 3680 mg/kg bw

Reliability : (2) valid with restrictions
1. The information was essentially confined to what is included in the current summary. No individual data were present.
2. Protocols were attached to the document, but they were not related to this test.
3. Only males were tested.

04.01.2002 (20)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type :
Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : oral feed
Exposure period : 90 days
Frequency of treatm. : daily
Post exposure period : None
Doses : 1.7-422 mg/kg bw/day
Control group : yes
NOAEL : = 23.7 mg/kg bw
Method : other: FIFRA 83-2
Year : 1978
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS:
- Species/strain: Fischer 344 rats
- Source: Charles River Breeding Laboratories Inc.
- Age: six weeks
- Weight at study initiation: male (130g), female (100g)
- Number of animals: 30/sex/dose group

ADMINISTRATION / EXPOSURE
- Exposure period: 90 days
- Route of administration: diet

- Post exposure period: none
- Doses: 0, 20, 80, 320, 1250, 2500, and 5000 ppm. which resulted in actual intakes of 1.5, 6.1, 23.7, 92.5, 191.8 and 401.7 mg/kg bw/day in males and 1.8, 7.4, 29.7, 116.0, 237.1 and 441.8 mg/kg bw/day in females

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical observation and mortality: Twice daily, detailed examination weekly
- Body weight: at baseline and weekly therafter
- Food consumption: weekly

CLINICAL CHEMISTRY:
In 10 animals/sex/dose group, at day 30 and at study termination;
- Hematology, hematocrit, hemoglobin, erythrocyte, count, mean corpuscular volume, total and differential leukocyte counts, platelet count, reticulocyte count.

- Biochemistry (in 10 animals/sex/dose group): at day 30 and at study termination; Serum lactate dehydrogenase (LDH), serum glutamic oxaloacetic transaminase (SGOT), serum glutamic pyruyic transaminase (SGPT), serum alkaline phosphatase, albumin, creatinine phosphokinase (CPK), glucose, blood urea nitrogen (BUN), direct bilirubin, total bilirubin, total cholesterol, globulin, indirect bilirubin, triglyceride, total protein, creatinine, calcium, uric acid, sodium, inorganic phosphorous, chloride, potassium.

- Urinalysis: specific gravity, pH, protein, glucose, ketones, bilirubin, urobilinogen, nitrite, hemoglobin and microscopic examination for cells or formed elements.

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights (at day 30 (10 animals/sex/dose) and at termination): liver, kidneys, heart, testes, and brain, including entire brain system.
- Macroscopic and microscopic (control and high dose group): eyes and the contiguous Harderian glands; heart; thyroid (with parathyroid); trachea; esophagus; stomach; adrenal glands; liver (with at least 2 lobes); kidneys; testes; ovaries; spleen; skin; sciatic nerve; mammary gland; gross lesions; bone (including marrow) taken from sternebrae, vertebrae or the tibio-femoral joint; spinal cord (at least 2 levels); any other target organ; a representative lymph node; lungs (2 coronal sections including all lobes and mainstem bronchi); lymph nodes; coronal sections (3) through the head (to include nasal cavity, paranasal sinuses, tongue, oral cavity, nasopharynx, and middle ear); brain (at least three levels from the forebrain, midbrain, and hindbrain); intestines (small and large) pancreas; skeletal muscle; urinary bladder; prostate; corpus and cervix uteri.

- residue analyses of liver, kidney, skeletal muscle, testes, mesentric adipose tissue, heart and one-half brain

ANALYSES:
- diet analyses for substance concentration

STATISTICAL METHODS:
- analysis of variance; Duncan's multiple range test

Result : CLINICAL OBSERVATIONS:
- Mortality and time of death: No rats died

- Clinical signs: dorsal hair loss in all groups

- Body weight gain: significantly decreased in both males and females at 2500 and 5000 ppm

- Food intake: intake in controls was statistically different from treated groups, no consistent positive or negative correlation however.

CLINICAL CHEMISTRY
- hematology: Males above 1250 ppm showed lower red blood cell counts, hemoglobin and hematocrit values and associated increase in number of reticulocytes, females at the two highest doses showed these signs to a lesser extent; reduced platelet counts over time (not treatment related)

- biochemistry: Males above 320 ppm showed signifficant depression of blood glucose at study termination, while females showed slight increase; inconsistent changes in serum triglycerides (not treatment related); at 5000 ppm both males and females showed elevated serum cholesterol; at 5000 ppm males showed significant decrease in serum protein at 30 days and at termination, for females significance only at 30 days; elevated albumin/globulin ratio at three highest doses (males) and highest dose (females); depressed serum calcium levels at 5000 ppm and increased phosphorus in males, in females to a lesser extent; elevated alkaline phosphatase and serum G/P transaminase at 5000 ppm in both sexes
indications of reduced renal function: significant increase in blood urea nitrogen in both sexes at 30 days for males at 2500 and 5000 persistent at 90 days; increased BUN/creatinine ration in males at 30 days but not at 90 days; significantly different values of uric acid for both sexes (without consistent trend)

- Urinalysis:
at 30 days: increased urobilinogen in males at 5000 ppm (other measures of bilirubin showed little deviation); slightly diminished protein excretion in both sexes at 5000 ppm; increased frequency of trace amounts of nitrite in males above 320 ppm
at 90 days: increased urobilinogen in both sexes at 2500 and 5000 ppm; decreased protein excretion with increasing dose in females for males only at 5000 ppm; increased frequency of trace amounts of nitrite in females at 2500 and 5000 ppm

MACRO- AND MICRSCOPIC FINDINGS
- Organ weights: significantly increased liver and kidney weight, both absolute and relative, in males above 320 ppm at 30 and 90 days (except at day 30 for 2500 ppm), females to a lesser extent at 2500 and 5000 ppm on day 30 and at 5000 ppm on day 90); sporadic deviation in heart and brain weight (no toxicological pattern); increased relative testis weight (not considered significant)
were a function of reduced overall body weight and are not considered significant.
- Macroscopy:
Interim kill - 30 Days:

control animals: diffuse brown discoloration of the kidney (1 male); enlargement of left mandibular lymph node (1 male);
5000 ppm: liver (diffuse dark staining) and kidney (cortex darkening or diffuse discoloration) discoloration in both males and females
90 days: no abnormalities in controls, at 5000 ppm dark brown discoloration of the liver and kidney (dark brown cortexes) in both males and females (females less affected)

- Histopathology:
Interim Kill - Day 30:
Presence of mononuclear cells in the lungs in both control and treatment group (not test substane related)
5000 ppm: increased liver cell hypertrophy in both sexes; increased mitotic figures in males and females (but to a lesser extent); liver tissue damage in both sexes
Terminal Kill - Day 90:
Both control and treatment group showed presence of mononuclear cells and vascular mineralization in the lung and cysts in various organs (all considered not treatment related);
Controls: cell death in liver in part of the males
5000 ppm: cell death and hypertrophy in liver cells of all males, in females only hypertrophy in part of the animals and no cell death; increased proliferation of oval cells and bile duct in majority of males; yellow pigmentation of Kupfer cells in all treated males

ANALYSES:
- In all cases diet formulation concentrations and test substance concentrations were within 10% tolerance limits

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (TACKLE 2AS formulation), purity 20-21.6%

Conclusion : NOAEL 320 ppm (23.7 mg/kg bw) based on the presence of liver damage with concomittant changes in blood chemistry

Reliability : (1) valid without restriction
21.05.2001 (12)

Type :
Species : rabbit
Sex : male/female
Strain : New Zealand white
Route of admin. : dermal
Exposure period : 21 days
Frequency of treatm. : 5 days/week
Post exposure period : None
Doses : 92, 277 and 923 mg/kg bw
Control group : yes, concurrent vehicle
NOAEL : = 277 mg/kg bw
LOAEL : = 92 mg/kg bw
Method : EPA OPP 82-2
Year :
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS:
- Species/strain: New Zealand white rabbits
- Source: H.A.R.E., Hewitt, NJ.
- Age: no data

- Mean Weight at study initiation: 2.59-2.64 (females), 2.65-2.68 (males)
- Number of animals: 10/sex/dose group

ADMINISTRATION / EXPOSURE
- Exposure period: 21 days
- Route of administration: dermal
- Post exposure period: none
- Doses: 92, 277 and 923 mg/kg bw, at day 4 highest dose was reduced to 4.62 mg/kg bw
- Vehicle: A NaOH solution (not specified) pH 7.5-7.6
- Total volume applied: 1ml, 3ml, 10ml (5ml after day 4)
- Area covered: 130cm2
- Occlusion: two layers of clean gauze plus occlusive binders for six hours
- Removal of test substance: after 6 hours

CLINICAL OBSERVATIONS AND FREQUENCY:
- Clinical signs: daily observation for external signs of toxicity. Dermal irritation readings according the method of Draize (1965) daily prior to application.
- Mortality: twice daily
- Body weight: day -1 thereafter the 4th and 7th day of the week, at sacrifice
- Food consumption: on day 1, 4, 7, 11, 14 and 21

CLINICAL CHEMISTRY
- Haematology: Total and differential leukocyte counts, erythrocyte count, hematocrit, hemoglobin, platelet count
- Biochemistry: alkaline phosphatase, urea nitrogen, glutamic pyruvate transaminase, glutamic oxaloacetate transaminase, calcium, potassium, lactic dehydrogenase, glucose, bilirubin (total and direct), total cholesterol, albumin, globulin, total protein
- Urinalysis: appearance, specific gravity, occult blood, protein, pH, bilirubin, urobilinogen, ketones, glucose, microscopic examination of formed elements

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Organ weights: adrenal glands, brain, heart, kidneys, liver, gonads, pituitary gland, thyroid and parathyroid.
- Macroscopic: abdominal cavity, abdominal wall, adipose tissue, adrenals, bladder, diaphragm, epididymes, gallblader, heart, large and small intestine, kidneys, liver, lungs, lymph nodes, mouth, nose, ovaries, pancreas, pituitary, salivary glands, sciatic nerve, skeletal muscle, treated and untreated skin, spleen, stomach, testes, thoracic cavity, thymus, thyroid, ureters, uterus and vagina
- Microscopic: treated and untreated skin, liver, kidneys and grossly abnormal tissue

ANALYSES:
-Method: HPLC analysis of test compound: isocratic 65% methanol/35% water 2ml/min on a waters radial compression system radial-pak A C18, detector 280nm.

- Sampling times: at study initiation and during week 1 and 2

STATISTICAL METHODS:
one-way analyses of variance (continuous data), Least

Significant Difference (differences among groupes), Mantel-Haenszel chi-square test (score data), chi-square with Yates correction (pathology data)

Remark : Tables with individual histopathological data are partly missing.

Result : CLINICAL OBSERVATIONS AND MORTALITY
- Mortality and time to death (day): at 923 mg/kg bw 19/20 died ore were sacrificed before day 8, one male survived until sacrifice; at 92 mg/kg bw 1 male (8); at 277 mg/kg bw 1 male (13); controls one male and one female (21)
- Clinical signs: at highest dose ataxia, decreased activity, nasal discharge, respiratory distress and salivation was seen in both sexes, males showed incidently diarrhoea and tremors; at 277 mg/kg bw incidental nasal discharge, hair loss, soft stool, tremors, diarrhoea and bloating was seen; at the lowest dose incidental signs were confined to diarrhoea and bloating; in all dose groups a white chrystaline substance at the application site was observed.
Severe dermal irritation with eschar formation was seen in males and females from day 2-3 to day 21 of exposure. A relationship with amount of applied material was evident.
- Body weight gain: decreased body weight in highest dose group (significant in females)
- Food/water consumption: individual low daily food consumption in high dose animals, significantly decreased on days 1-4

CLINICAL CHEMISTRY
No treatment related effects

MACRO- AND MICROSCOPIC FINDINGS
- Organ weights: at 277 mg/kg bw significant increase in mean relative adrenal weight in females (toxicological significance questionable)
- Macroscopy: marked dermatitis with epithelial necrosis and eschar formation at the exposure site for all exposure levels.
- Histopathology: microscopic changes indicative of macroscopic findings, all other findings were incidental and not related with treatment. Effects on intestinal epithelium were attributed to coccidal infections

ANALYSES:
- Actual dose was 87-106% of nominal value
- Stability: ok
- Homogeneity: ok

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : CAS 62476-59-9 (Acifluorfen, sodium salt), purity: technical acifluorfen was dissolved in 0.82 M NaOH yielding a preparation of 240 mg/ml liquid

Conclusion : Tackle 2S was acutely toxic when administered at the high dose. Body weight gain and food consumption were decreased in high dose animals. Nineteen of 20 animals receiving the high dose did not survive past day eight of the study. In addition Tackle 2S was a severe cumulative dermal irritant at all dose levels. No toxicologically significant changes in body weight, food consumption, hematological and clinical chemistry parameters, or urinalysis data were observed among control, low dose, and mid dose groups.
NOAEL systemic 277 mg/kg based on survival and body weight

		LOAEL local effects 92 mg/kg
Reliability	:	(2) valid with restrictions 1. limited histopathology 2. effect on adrenal weight is questionable

21.05.2001 (11)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Cytogenetic assay
System of testing	:	CHO cells
Test concentration	:	0.5-5.0 ul/ml
Cycotoxic concentr.	:	
Metabolic activation	:	without
Result	:	negative
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	- Species/cell type: Chinese hamster ovary cells - Metabolic activation system: none - No. of anaphases analyzed: 300 ADMINISTRATION: - Doses: 0.5, 1.0 and 5.0 ul/ml - Exposure period: 3 hours - Positive and negative control groups and treatment: Positive control was Ethylmethanesulfonate (EMS) and was added at 0.5 µ1/ml; spontaneous controls were also maintained. CRITERIA FOR EVALUATING RESULTS: - assesment of mitotic spindle damage by screening cells microscopically for multinuclei or anaphase bridges - Statistical method: Chi square analysis
Result	:	GENOTOXIC EFFECTS: - Without metabolic activation: none PRECIPITATION CONCENTRATION: no details given. CYTOTOXIC CONCENTRATION: no information available STATISTICAL RESULTS: There was no significant difference between controls and test samples regarding mititic spindle damage.
Source	:	Notox Hertogenbosch Toxicology and Regulatory Affairs Flemington NJ
Test substance	:	CAS 62476-59-9 (sodium 5-(2-chloro-4-trifluoro-methylphenoxy) 2-nitrobenzoate), purity not indicated
Reliability	:	(3) invalid 1. No standard study type; pilot study

21.05.2001 (13)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Cytogenetic assay
Species	:	mouse

Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	single dose
Doses	:	0, 100, 500, 1000 mg/kg.
Result	:	negative
Method	:	OECD Guide-line 475 "Genetic Toxicology: In vivo Mammalian Bone Marrow Cytogenetic Test - Chromosomal Analysis"
Year	:	1986
GLP	:	yes
Test substance	:	other TS

Method :

TEST ORGANISMS:
- Strain: Crl:CD-1(ICR)BR mice
- Source: Charles River Kingston Breeding Laboratories (Stoneridge, New York)
- Age: no data
- Weight at study initiation: 18.5 - 28.5 g
- No. of animals per dose: 15/sex/dosage

ADMINISTRATION:
- Vehicle: distilled water
- Doses: Test compound: 0, 100, 500, 1000 mg/kg by gavage. The corresponding dose levels based on active ingredient are 0, 42.8, 214, 428 mg/kg, respectively.
- Duration of test: The in-life portion of the study was 3 days. Ten animals of each dose group were killed 6, 27, and 51 hr after dosing.
- Frequency of treatment: single dose by oral gavage
- volume 10 ml/kg.
- Control groups and treatment:
Negative control: vehicle 15 animals per sex.
Positive control: Triethylmelamine, ip 0.3 mg/kg (5 animals per sex).
- number of metaphases scored: 50/animal

EXAMINATIONS:
- Clinical signs and mortality: daily.
- Body weight: daily for 4 days (separate group of 8 animals)

CRITERIA FOR EVALUATING RESULTS:
- no. of cells with aberrations per 5 animals

STATISTICAL ANALYSIS: The Beta-binomial model (Stiratelli et al., 1985)

Result :

MORTALITY: none

CLINICAL SIGNS:
Yellow stained anogenital area, passiveness, ruffled fur, and abdominal breathing were observed after treatment with 428 mg/kg test material and at a lower incidence at 214 mg/kg test material. Recovery was observed. Abnormal toxic signs were not observed in the animal positive control, distilled water control groups or test material 42.8 mg/kg treatment group prior to sacrifice.

BODY WEIGHT CHANGES: no effect

GENOTOXIC EFFECTS: No. of cells with aberrations at 6, 27 and 51 hours 11, 11 and 12 respectively (12, 11 and 5 in vehicle controls)

POSITIVE CONTROL: A significant increase in the frequency of bone marrow chromosomal aberrations and an increase in translocations and rearrangements

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (Acifluorfen, sodium salt), purity 42.8%

Conclusion : Negative, solvent and positive controls were within the expected ranges.

Reliability : (2) valid with restrictions
1. Only slides of 1000 mg/kg were scored for genotoxic effects. Slides of the lower dose groups were not examined because an effect did not occur at the highest dose group.
2. Only 50 metaphases per animal were scored (100 according to OECD 475)

21.05.2001 (19)

5.8.1 TOXICITY TO FERTILITY

Type : Two generation study
Species : rat
Sex : male/female
Strain : other: Crl:COBS-CD-(SD)BR
Route of admin. : oral feed
Exposure period : Parent/F1-generation (males/females): 12 weeks before cohabitation for mating until completion of a 3-week cohabitation period for males or until day 25 of presumed pregnancy (non-pregnant females) or day 21 of lactation (pregnant females)
Frequency of treatm. : continuous
Premating exposure period
Male : 12 weeks
Female : 12 weeks
Duration of test : 42 weeks (maximum): Parent/F1-generation; 12 weeks premating/treatment, 3 weeks cohabitation, 3 weeks pregnancy, 3 weeks lactation
No. of generation studies :
Doses : 25, 500 and 2500 ppm in the diet
Control group : other: diet without the test substance
NOAEL parental : = 25 ppm
NOAEL F1 offspring : = 500 ppm
NOAEL F2 offspring : = 500 ppm
Method : other: US EPA, Pesticide Assessment Guideluines, Subdivision F, Hazard Evaluation: Human and Domestic Animals.
Year : 1982
GLP : yes
Test substance : other TS

Method :

TEST ORGANISMS
- Age: males/females (parental generation) 7 weeks at start treatment
- Source: Charles River Breeding Laboratories Inc., Kingston, NY
- Weight at study initiation: At start treatment males 177-238g and females 123-169g
- Number of animals: 35/sex/treatment (parent), 40/sex/treatment (F1)

ADMINISTRATION / EXPOSURE

- Test duration: maximum 39 weeks
- Exposure period: males (parent/F1 generation) 12 weeks prior to mating and maximal 3 weeks cohabitation; Females (parent generation) 12 weeks prior to mating, maximal 3 weeks cohabitation, 3 weeks pregnancy and 3 weeks lactation Females (F1-generation) after weaning 12 weeks prior to mating, maximal 3 weeks cohabitation, 3 weeks pregnancy and 3 weeks lactation
- Route of administration: oral via the diet
- Doses: 0, 25, 500 and 2500 ppm in the diet (actual exposure in terms of the average mg/kg/day dosage was calculated to be higher in females than in males for each generation and within each sex the second generation received higher mg/kg/day dosages than the first generation)

MATING PROCEDURES:
- Mating: 1 female / 1 male
- Day 0 of gestation: presence of copulation plug and/or spermatozoa in the vaginal smear of females

PARAMETERS ASSESSED DURING STUDY:
- Mortality: mimimum of twice each day
- Clinical observations: daily during exposure
- Body weight gain: at least once weekly during exposure, during gestation on day 0, 6, 10, 15, 20 and 25, during lactation on day 1, 4, 7, 11, 14, 16, 18 and 21
- Food consumption: at least once weekly during exposure, during gestation on day 0, 6, 10, 15, 20 and 25, during lactation on day 1, 4, 7, 11, 14, 16, 18 and 21
- Female oestrous cycle: vaginal cytology examination during cohabitation and until confirmation of pregnancy (maximum 3 weeks)
- Mating and fertility data (males/females): days in cohabitation, number of males/females mated/not mated, number of successful matings , time between pairing and mating (with 1rst or 2nd male)
- Maternal behaviour (dams which delivered): during the 3-week lactation period when examining the pups
- Maternal delivery data: duration of gestation, number pregnant and surviving delivery, number surviving with still borns, litter size (live and dead pups), number and placements of implants at sacrifice (day 21 of lactation)
- Pup viability: vital status at birth (live or stillborn) and at least twice daily viability until culling (day 4 post-partum for the parent generation, maximum 8 pups/litter) or weaning (day 21 post-partum for the parent/F1-generation)
- Pup observations: physical signs (including nursing behaviour and gross external anomalies) daily during lactation; body weights on days 1 (birth), 4, 7, 14 and 21 of lactation

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopy: all males and females (parental generation) and those selected for pairing (F1-generation) were necropsied and gross findings recorded and all gross lesions, target organs (liver, kidney and stomach), pituitary gland and reproductive organs (males: testes, epididymides, seminal vesicles, prostate and coagulation gland and females: vagina, uterus, cervix, ovaries and mammary gland) were removed and preserved in fixative. All

pups, except those precluded by autolysis or cannibalism, were necropsied and examined for gross lesions. Additionally, at weaning the heads of pups (except those selected for pairing) were cross-sectioned for examination of hydrocephaly
- Microscopy: histopathology examinations were preformed on the kidney, stomach and gross lesions of rats of the parental generation and on gross lesions of pups of the F1 and F2 generations). The reproductive organs, liver and pituitary gland were examined from 20 selected males and females of the control and high dosage groups of the parental and F1 generations

ANALYSES:
- Method: HPLC/UV
- Sampling time: weekly (accuracy of preparation) and on days 0, 1, 4, 7, 10, 14 and 21 (stability and homogeneity)

STATISTICAL METHODS: Bartlett's test, Analysis of variance, Dunnett's test, Kruskal-Wallis test, Dunn's test, Analysis of covariance, Covariance Analysis T-test, Variance test for the Homogeneity of the Binomial Distributi

Result :

ANALYSES:
- Actual dose level: the accuracy of all test diets was acceptable (within 15% of nominal concentrations); in control diet from week 26 onwards significant amounts of test substance (compared to the low dose level) were found
- Stability: stable for at least 21 days (mean recovery 82-91%)
- Homogeneity: homogeneous (first batch recovery 72-120%, two samples at 250 ppm (mid) 131 and 184%; second batch 84-113%)

ACTUAL INTAKE (mg/kg bw):
Males premating (P/F1):
at 50, 500 and 2500 ppm, 1.5-1.7, 29-33 and 147-169 mg/kg bw resp..
Females premating (P/F1):
at 50, 500 and 2500 ppm, 1.8-1.9, 29-38, 153-199 mg/kg bw resp..
Females pregnancy (P/F1)
at 50, 500 and 2500 ppm, 1.5-1.6, 29-30, 153-157 mg/kg bw resp..
Females Lactation (P/F1):
at 50, 500 and 2500 ppm, 2.9-3.2, 57-61, 252-287 mg/kg bw resp..

TOXIC EFFECTS BY DOSE LEVEL

PARENTAL GENERATION:

- Mortality: at 25 ppm one female and at 2500 ppm one male
- Body weight: at 2500 ppm decreased in males and females and at 500 ppm increased in females during lactation only
- Food consumption: at 500 ppm decreased in females (day 6-15 of gestation) and at 2500 ppm decreased in males and in females during lactation
- Clinical signs: at 2500 ppm increased chromodacryorrhoea and urine stained abdominal fur in males and emaciation in females
- Mating and fertility data (males/females): no differences

between the dose groups; at 0, 50, 500 and 2500 ppm 30, 29, 31 and 32 females pregnant
- Maternal delivery data: no treatment related effects on duration of gestation, surviving dams/pups; at 2500 ppm decreased number of implantations sites
- Pup data: no differences between the dose groups considering viability and sex ratio: at 2500 ppm decreased pup weights between birth and day 21 post-partum
- Macroscopic examinations: very low incidences of mottled appearance of the renal pelvis in males at 500 and 2500 ppm; stomach with dark red to black areas in females at 2500 ppm
- Microscopic examinations: at 500 and 2500 ppm kidney lesions characterised by dilation of tubules in the outer medulla of females

F1 GENERATION:

- Mortality: at 0 ppm one female, 25 ppm one male and 2500 ppm one male and 5 females
- Body weight: at 2500 ppm decreased in males and females
- Food consumption: at 2500 ppm increased in males and females
- Clinical signs: at 2500 ppm thin or emaciated and/or weak appearance, chromorrhinorrhoea and urine stained fur among males and thin appearance among females
- Mating and fertility data (males/females): no differences between the dose groups; no of mated/pregnant femles 35/28, 36/29, 37/27 and 39/35 at 0, 50, 500 and 2500 ppm resp.
- Maternal delivery data: at 2500 ppm decreased duration of gestation; no effects on implantation sites and number of surviving dams/pups
- Pup data: no differences between the dose groups considering sex ratio; at 500 and 2500 decreased viability on days 1 and 4 post-partum
- Macroscopic examinations: at 2500 ppm kidney lesions consisting of dilated renal pelvis in males and white/brown raised areas in females and gastric lesions (black areas) in females
- Microscopic examinations: at 500 and 2500 ppm kidney lesions characterised by dilation of tubules in the outer medulla in females and an increased incidence of pelvic dilatation in males

F2 GENERATION:

- Clinical signs: at 2500 ppm thin and weak appearance and cannibalism of ears (partially) and tail tip
- Pup effects: at 500 and 2500 ppm one litter died after day 2 or day 5 post-partum, respectively; at 2500 ppm body weight was decreased
- Macroscopic examinations: at 2500 ppm gross kidney lesions consisting of slight/moderate dilation of the kidney pelvis

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9 (Acifluorfen sodium salt, technical grade), purity not reported

Conclusion : NO(A)EL (parental): 25 ppm, based on an increased incidence of kidney lesions (dilated tubules in the outer medulla) in the 500 and 2500 ppm group. Additional findings in the 2500 ppm group consisted of decreased body weight
NO(A)EL (developmental): 500 ppm, based on reduced pup body weights and an increased incidence of kidney pelvic

dilatation

Reliability : (1) valid without restriction
21.05.2001 (1)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	other: Crl:COBS-CD-(SD)BR
Route of admin.	:	gavage
Exposure period	:	gestation days 6-19
Frequency of treatm.	:	daily
Duration of test	:	Caesarean sections on gestation day 20
Doses	:	20, 90 and 180 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 20 mg/kg bw
NOAEL teratogen.	:	= 20 mg/kg bw
NOAEL Fetotoxicity	:	= 20 mg/kg bw
Method	:	other: EPA; Hazard Evaluation: Humans and Domestic Animals, Federal Register. Part II, Vol. 43, no. 163.83-3
Year	:	1978
GLP	:	yes
Test substance	:	other TS

Method :

TEST ORGANISMS
- Age: females 12 weeks (at start mating procedures)
- Weight at study initiation: 211-255g (gestation day 0)
- Number of animals: 25 (treatment/control groups)
- Source: Charles River, Breeding Laboratories, Inc.

ADMINISTRATION / EXPOSURE
- Test duration: 20 days
- Exposure period: gestation days 6-19
- Route of administration: oral gavage
- Doses: 0, 20, 90 and 180 mg/kg
- Total volume applied: 10 ml/kg
- Vehicle: water (reverse osmosis)

MATING PROCEDURES:
- Mating: 1 female / 1 male
- Day 0 of gestation: presence of copulation plug

PARAMETERS ASSESSED DURING STUDY:
- Mortality/clinical observations: gestation days 0 and 20 and several times per day on gestation days 6-19
- Body weight gain: gestation days 0 and 20 and daily during treatment (gestation days 6-19)
- Food consumption: not measured
- Maternal reproduction parameters (general): Number of pregnancies and corpora lutea
- Examination of uterine content: number and distribution of implantations, early and late resorptions and live and dead foetuses
- Examination of fetuses: sex; weight; external, visceral (1/3) and skeletal (2/3 foetuses) findings

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopy: all females
- Microscopy: gross lesions (preliminary deaths) preserved

for possible histopathology

ANALYSES:
- Method: HPLC
- Sampling time: weekly samples taken for possible analysis

STATISTICAL METHODS: Bartlett's test, Analysis of Variance, Analysis of Covariance, aproximate test of equality of means, Dunnett's test, Kruskal-Wallis, Dunn's method of multiple comparisons

Result : ANALYSES:
- Actual dose level: not reported
- Stability: Not reported

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:

- Mortality and day of death: at 180 mg/kg 3 females died on gestation days 10 or 17
- Body weight: at 180 mg/kg decreased during treatment (gestation days 9-19) and overall gestation days 6-19 and 0-20
- Clinical signs: females showed at 90 mg/kg excessive salivation and at 180 mg/kg excessive salivation, vocalization, hyperactivity, impaired/lost righting reflex, decreased motor activity, chromodacryorrhoea, rales, urine stained abdominal fur and chromorrhinorrhoea
- Number pregnant per dose level: at 0, 20, 90 and 180 mg/kg, 22, 21, 19, 24, respectively
- Number aborting: none
- Number of resorptions (early/late): at 0, 20, 90 and 180 mg/kg, 0.95 (7.3%), 0.90 (6.6%), 1.42 (10.4%) and 2.20 (16.2%), respectively (percent of implantation sites)
- Number of implantations: at 0, 20, 90 and 180 mg/kg, 13.1, 13.6, 13.7 and 13.6, respectively
- Number of corpora lutea: at 0, 20, 90 and 180 mg/kg, 14.7, 14.7, 15.4 and 14.6, respectively
- Duration of Pregnancy: scheduled sacrifice on gestation day 20
- Gross pathology incidence and severity: no findings in surviving females. In 2 out of 3 females found dead (180 mg/kg) erosions in the mucosa of the stomach or haemorrhagic lungs were noted

FETAL DATA:

There were no gross external, soft tissue or skeletal alterations that were considered effects of the test substance. Variations noted in soft tissue examinations and in skeletal ossification were correlated with lower foetal body weights

- Litter weights (gravid uterus): not recorded
- Number viable: at 0, 20, 90 and 180 mg/kg, 12.2, 12.7, 12.3 and 11.4, respectively
- Sex ratio (percentage of males): at 0, 20, 90 and 180 mg/kg, 51.1%, 54.3%, 48.1% and 46.9%, respectively
- Body weight (gain): at 0, 20, 90 and 180 mg/kg, for males 3.8g, 3.87g, 3.5g and 3.09g, respectively and for females 3.62g, 3.64g, 3.30g and 2.97g, respectively.
- Grossly visible abnormalities: no findings associated with treatment
- Visceral abnormalities: at 90 and 180 mg/kg increased

incidence of slight dilation of the lateral ventricles of the brain
- Skeletal abnormalities: at 90 and 180 mg/kg delayed ossification of metacarpals, forepaw phalanges and hindpaw phalanges and additionally in 180 mg/kg group litters delayed ossification of the caudal vertebrae, sternebrae and metatarsals

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9, purity 91.2%

Conclusion : NOAEL (maternal): 20 mg/kg, based on decreased body weights, clinical signs such as excessive salivation in the 90 and 180 mg/kg groups and mortality and clinical signs including vocalization, huperactivity, impaired righting reflezx, decreased motor activity, chromodacryorrhoea, rales, urine stained abdominal fur, chromorrhinorrhoea in the 180 mg/kg group
NOAEL (teratogenicity): 180 mg/kg
NOAEL (foetotoxicity): 180 mg/kg

Reliability : (1) valid without restriction
19.02.2003 (3)

Species : rabbit
Sex : female
Strain : New Zealand white
Route of admin. : gavage
Exposure period : gestation days 6-29
Frequency of treatm. : Once daily
Duration of test : Caesarean sections on gestation day 30
Doses : 3, 12 and 36 mg/kg
Control group : yes, concurrent vehicle
NOAEL maternal tox. : = 12 mg/kg bw
NOAEL teratogen. : = 36 mg/kg bw
NOAEL Fetotoxicity : = 12 mg/kg bw
Method : other: EPA, federal register, 1978, Part II, Vol. 43, No. 163, 163.83-3
Year : 1978
GLP : yes
Test substance : other TS

Method : TEST ORGANISMS
- Age: females (at insemination) 26 weeks
- Weight at study initiation: 3.06-5.13 kg
- Number of animals: 16 (treatment/control groups)
- Source: Dutchland Laboratories Inc., Denver Pennsylvania, USA

ADMINISTRATION / EXPOSURE
- Test duration: 309 days
- Exposure period: gestation days 6-29
- Route of administration: oral gavage
- Doses: 0, 3, 12 and 36 mg/kg/day
- Vehicle: water (revers osmosis)
- Dose volume: 10 mg/kg/day

MATING PROCEDURES:
- Artificial insemination: Semen collected from 4 proven donor bucks of the same strain and source as the females. 3 hours before insemination females were intravenously injected with 20 USP units/kg of Human Chorionic Gonadotropin. Insemination of 0.25 mL of diluted (with saline) semen sample (6.0 million spermatozoa/0.25 mL)
- Day 0 of gestation: day of insemination

PARAMETERS ASSESSED DURING STUDY:
- Mortality: several times/day during treatment (gestation days 6-29) and on gestation day 30
- Clinical observations: On gestation day 0 and several times/day during treatment (gestation days 6-29) and on gestation day 30
- Body weight gain: once daily on gestation days 0 and 6-30
- Food consumption: once daily on gestation days 0 and 6-30
- Examination of uterine content: number of corpora lutea; number and distribution of implantations, early and late resorptions and live and dead foetuses
- Examination of fetuses: sex; weight; external, visceral (all foetuses) and skeletal (all foetuses) findings; brains being subjected to a variation of Staple's technique

ORGANS EXAMINED AT NECROPSY (MACROSCOPIC AND MICROSCOPIC):
- Macroscopy: findings all dams recorded, all gross lesions (except commonly found parovarian cysts) were fixed for possible histopathology
- Microscopy: not performed

ANALYSES:
- Method: not indicated (analysis separately by the sponsor)
- Sampling time: weekly samples taken

STATISTICAL METHODS: Bartlett's Test, Kruskal-Wallis Test and Fisher's Exact Test

Result : ANALYSES:

Data on the accuracy and stability of preparations were kept on file with the sponsor

- Actual dose levels: reported as being correct
- Stability: no results presented
- Homogeneity: not determined (solutions)

MATERNAL TOXIC EFFECTS BY DOSE LEVEL:

- Mortality and day of death: at 0 mg/kg three females died or were sacrificed (2 following an intubation error, 1 following abortion), at 3 mg/kg one female was sacrificed because of a back injury and at 12 mg/kg one female was sacrificed following abortion
- Body weight: at 36 mg/kg slightly inhibited body weight gain on gestation days 6-18 and overall inhibition of body weight gain during gestation days 6-30
- Food consumption: at 36 mg/kg marked inhibition of food consumption during gestation days 23-24. Recovery of food consumption during gestation days 29-30
- Clinical signs: no treatment-related signs
- Number pregnant per dose level: 13 (81.2% of number inseminated), 13 (81.2%), 12 (75.0%) and 11 (68.8%) in the 0, 3, 12 and 36 mg/kg group, respectively
- Number aborting: at 0 mg/kg one female and at 12 mg/kg one female
- Natural deliveries: at 0, 3, 12 and 36 mg/kg, 1, 2, 2 and 2, respectively
- Number of resorptions (early/late): at 0, 3, 12 and 36 mg/kg, 0.6, 0.4, 0.7 and 0.7, respectively
- Number of implantations: at 0, 3, 12 and 36 mg/kg, 6.8,

7.2, 7.3 and 9.0, respectively
- Post implantation loss: not calculated
- Number of corpora lutea: at 0, 3, 12 and 36 mg/kg, 9.3, 9.7, 10.7 and 11.1, respectively
- Duration of Pregnancy: scheduled sacrifice on gestation day 30
- Gross pathology incidence and severity: at 36 mg/kg, increased incidence of involuted ovaries combined with congested uterus in 4 females

FETAL DATA:

There were no gross external, soft tissue or skeletal alterations that were considered effects of the test substance.

- Litter size: 0, 3, 12 and 36 mg/kg, 6.2, 6.8, 6.7 and 8.3, respectively
- Number viable: at 0, 3, 12 and 36 mg/kg, 6.2, 6.8, 6.7 and 8.3, respectively
- Sex ratio (percentage of males): at 0, 3, 12 or 36 mg/kg, 50.0%, 51.5%, 55.9% and 48.0%, respectively
- Body weight: at 0, 3, 12 and 36 mg/kg, 51.3g, 47.4g, 53.3g and 43.1g, respectively
- Grossly visible abnormalities: no treatment related findings
- Visceral abnormalities: incidental findings comprised accessory spleen, agenesis of the gall bladder and malformation of the diaphragm with atelectasis
- Skeletal abnormalities: incidentally observed findings consisted of rudimentary rib (between R5-6), fused rib (L6-7), 1 or more fused sternebrae, 1-4 asymmetric sternebrae, stubbed tail and split xiphoid vertebral

Source : Notox Hertogenbosch
Toxicology and Regulatory Affairs Flemington NJ

Test substance : III, CAS 62476-59-9, Concentration 240 mg/ml in water (activity 22.4%), purity 81.2%

Conclusion : NOAEL (maternal): 12 mg/kg, based on slight inhibition of body weight gain and marked inhibition of food consumption
NOAEL (teratogenicity): 36 mg/kg
NOAEL (foetotoxicity): 12 mg/kg, based on possible interference with implantations and slight decrease of foetal body weights

There were no differences noted among the dose groups in the number of corpora lutea, implantations, litter sizes, early and late resorptions, foetal sex ratio, number of resorbed conceptuses and number of does with any resorptions. The increased number of involuted corpora lutea and congested mucosa in the uteri may be attributed to interference of the test substance with implantation after fertilization (nidation of fertilized eggs in rabbits approximately gestation day 8)

Reliability : (2) valid with restrictions
Only 9-10 litters per dose group evaluated

21.05.2001 (2)

(1) Argus Research laboraties, Inc., Reproductive Effects of Tackle Administered orally in Feed to Crl:COBS-CD-(SD)BR Rats for Two Generations, 1986

(2) Argus Research Laboratories, Inc, Teratogenic potential of TACU 06238001 in New Zealand White Rabbits (segment II Evaluation), 1980 (76)

(3) Argus Research Laboratories, Inc., Teratogenicity Study of TACU 06238001 in Pregnant Rats, 1981

(4) BASF, Acifluorfen-sodium - determination of vapor pressure (1990) (84)

(5) BASF, Determination of acifluorfen sodium solubility in water and organic solvents (1991) (83)

(6) BASF, Determination of aciflurofen sodium octanol/water partition coefficient (1991) (82)

(7) BASF, Phase 3 Summary of Accession #095735 A Hydrolysis Study with 14C-RH-6201: Technical Report #3423-75-66 (1990) (86)

(8) EFED Ecological Risk Assessment for sodium acifluorfen. US EPA, Registration Process Documents, June 2000. http://www.epa.gov/pesticides/reregistration/acifluorfen/efedhapter.pdf

(9) EFED Ecological Risk Assessment for sodium acifluorfen. US EPA, Registration Process Documents, June 2000. http://www.epa.gov/pesticides/reregistration/acifluorfen/efedhapter.pdf p 71

(10) EPIWIN v3.05, Syracuse Research Corporation, Syracuse, NY (July 12, 2000)

(11) Food and Drug Research Laboratories, Subchronic 21-day dermal toxicity study in rabbits, 1981

(12) Gulf South Research Institute, Evaluation of ninety day subchronic toxicity to 'Tackle' in Fischer 344 rats, 1981

(13) Mobil Environmental and Health Science Department, Anaphase analysis of CHO cells treated in vitro with Tackle 2S, 1981.

(14) Mobil Oil Corporation, Acute toxicity of 10318001 to rainbow trout (Salmo gairdneri), 1981 (79)

(15) Mobil Oil Corporation, Acute toxicity of 10318001 to the bluegill (Lepomis macrochirus), 1981 (78)

(16) Mobil Oil Corporation, Acute toxicity of 10318001 to the water flea (Daphnia magna), 1981 (77)

(18) Rhone-Poulenc Ag Company, Acifluorfen-sodium - determination of melting point (1990) (81)

(19) Rohm and Haas Company, BLAZER herbicide in vivo cytogenetic study in mice, 1987 (69)

(20) Rohm and Haas, Research Division, Single dermal dose with (experimental) Herbicide RH 6201, Aqueous technical, 39.6% a.i., 1976 (67)

(21) Rohm and Haas, Research Division, Single oral dose with (experimental) Herbicide RH 6201, Aqueous technical, 39.6% a.i., 1976 (67)

(22) Toxigenics, Inc., Four-hour acute aerosol inhalation toxicity study in rats of Tackle 2AS Herbicide, 1980 (68)