201-14870B

APPENDIX

Robust Summaries for Substances in the HPV Test Plan for the Monoesters Category of the Aliphatic Esters Chemicals

Part I. HPV Substances in the Monoesters Category
Part II. Surrogate Monoesters

November 26, 2003

Appendix -Robust Summaries for Aliphatic Esters - Monoesters HPV Test Plan

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Part I - Robust Summaries for HPV Substances in the Monoesters Category of Test Plan

HPV Monoesters Substances
identified by CAS Numbers and as organized in Table 1B of the HPV Test Plan

Part II - Robust Summaries for Surrogate Monoesters

Six Surrogate Monoesters Substances

- Stearic acid, butyl ester (CAS No. 123-95-5)
- Fatty acids, C16-18 saturated and C18-unsaturated, 2-ethylhexyl ester (CAS No. 85049-37-2)
- Stearic acid, octyl ester (CAS No. 109-36-4)
- Oleic acid, decyl ester (CAS No. 3687-46-5)
- Stearic acid, myristyl ester (CAS No. 17661-50-6)
- Stearic acid, isocetyl ester (CAS No. 25339-09-7)

PART I. HPV Substances in the Monoesters Category

Acute Oral Toxicity (CAS No. 29806-73-3)

Test Substance	Palmitic acid, 2-ethylhexyl ester
CAS Number	29806-73-3
Remarks	Purity not specified
Method/guideline	Not indicated
Test type	Acute oral toxicity
GLP	Yes, reportedly met FDA, TSCA, FIFRA guidelines
Year	1982
Test system	Species (Strain) Rats (Wistar), weight 213 - 230 g Sex: Male No. of animals: 10 males/treatment Route: Oral gavage Dosage: 5000 mg/kg body weight, single oral dose to fasted rats Statist. Methods: No specified.
Test conditions	Single oral administration of 5000 mg/kg bw; no controls; feeding *ad libitum* but food was withheld ~16-20 h prior to dosing. Animals were observed for mortality and clinical symptoms 3-4 hrs after dosing and once daily thereafter for 14 days.
Results/Remarks	Nine of the ten animals survived the 5 g/kg oral dose. One rat died on day 1. Instances of lethargy, piloerection, ptosis, chromodacryorrhea, diarrhea, ptosis as well as wetness of the anogenital area were noted as minor effects/observations during the study.
Conclusions	The acute oral LD_{50} for the test substance was > 5 g/kg in rats.
Data Quality	Reliable with restrictions. [Klimisch reliability 2]. Necropsy was not performed at the end of the 14 day period.
References	1) Confidential business information. 2) Findings have also been cited by Elder RL (1982). Final report on the safety assessment of octyl palmitate, cetyl palmitate and isopropyl palmitate, J. Amer. Coll. Toxicol. **1(2):** 13-35.
Other	Date last updated: November 11, 2003.

Acute Oral Toxicity (CAS No. 68334-13-4)

Test Substance	Fatty acids, tall oil, 2-ethylhexyl ester
CAS Number	68334-13-4
Remarks	Purity not specified
Method/guideline	Not indicated
Test type	Acute oral toxicity
GLP	No
Year	1972
Test system	Species (Strain) Rat, weight 200-300 g Sex: Male and female No. of animals: 5/treatment Route: Oral gavage Dosage: Undiluted at dose of 2.0, 4.0, 8.0, 16.0, 32.0 or 64.0 ml/kg body weight

Test conditions	Single oral (gavage) administration of 2, 4, 8, 16, 32 or 64 ml/kg body weight; no controls; feeding *ad libitum* but food was withheld ~24 h prior to dosing. Mortality/clinical signs daily for 14 days. Each dose level consisted of 5 animals. Males and females were indicated to be distributed equally. No measurements of body weights or post-mortem investigation were performed.
Results/Remarks	No deaths were reported in any of the dose groups at the end of the 14-day observation period. Animals dosed with 8 ml/kg and below did not exhibit any adverse effects. At 16 ml/kg and the 32 ml/kg dose levels, sluggish and impaired locomotion as well as wet unkempt coats were noted in the rats. At the 64 ml/kg oral dose, animals exhibited sluggish and impaired locomotion, swelling around the ocular area and wet, messy coats. Slight loss of hair was noted after the 4th day. Behavior patterns and eating habits remained normal in all animals.
Conclusions	The acute oral LD_{50} was > 64.0 ml/kg body weight
Data Quality	Reliable with restrictions. [Klimisch reliability 2]. Not GLP. No post-mortem or histopathology examinations were performed.
References	Unpublished confidential business information.
Other	Date last updated: November 11, 2003.

Part II. Surrogate Monoesters

Melting Point (CAS No. 123-95-5)

Test Substance **CAS Number** **Remarks**	Stearic acid, butyl ester 123-95-5 Purity not specified
Method/guideline	Not specified
Test type **GLP** **Year**	Melting point Not specified 1972
Remarks	Method of melting point determination was not given. Physical chemical property was cited in Handbook of Chemistry and Physics
Conclusions	Melting Point 27.5 °C
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature.
References	Handbook of Chemistry and Physics. R.C. Weast (ed.). 53 rd Ed., CRC, Cleveland OH, pg. C-265 (1972)
Other	Date last updated November 10, 2003.

Boiling Point Point (CAS No. 123-95-5)

Test Substance **CAS Number** **Remarks**	Stearic acid, butyl ester 123-95-5 Purity not specified
Method/guideline	Not specified
Test type **GLP** **Year**	Boiling Point Not specified Not specified
Remarks	Method of boiling point determination was not given. Physical chemical property was cited in Merck Index
Conclusions	Boiling Point 343 °C
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature.
References	M. Windholz (ed.). Merck Index (Ninth Ed.). pg. 202, Merck & Co., Rahway, NJ (1976)
Other	Date last updated November 10, 2003.

Vapor Pressure (CAS No. 123-95-5)

Test Substance	Stearic acid, butyl ester
CAS Number	123-95-5
Remarks	Purity not specified
Method/guideline	Not specified.
Test type	Vapor pressure
GLP	Not specified
Year	1972
Remarks	Method of vapor pressure determination was not given. Physical chemical property was cited in review article by Elder (1985)
Conclusions	Vapor pressure: 11 mm Hg (150 °C)
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature.
References	Elder RL (1985). Final report on the safety assessment of butyl stearate, cetyl stearate, isobutyl stearate, isopropyl stearate, myristyl stearate and octyl stearate , J. Amer. Coll. Toxicol. **4(5):** 107-146.
Other	Date: November 10, 2003.

Acute Oral Toxicity (CAS No. 123-95-5)

Test Substance	Stearic acid, butyl ester
CAS Number	123-95-5
Remarks	Purity not specified
Method/guideline	Not indicated
Test type	Acute oral toxicity
GLP	No
Year	1953
Test system	Species (Strain) Rat (not specified) Sex: Male No. of animals: 6 or 15 males/treatment Route: Oral gavage Dosage: 4, 8, 16 and 32 g/kg body weight undiluted
Test conditions	Undiluted butyl stearate was administered in single oral doses of 4, 8, 16 and 32 g/kg body weight to 4 groups of male rats consisting of 6, 15, 6 and 15 animals, respectively. Statistical methods were not specified.
Results/Remarks	Smith (1953) reported that no deaths or gross lesions or pathological changes at any of the doses tested. The test material was well tolerated by the rats.
Conclusions	The acute oral LD_{50} was > 32 g/kg in rats.
Data Quality	Reliable with restrictions [Klimisch reliability 2]. Not GLP. Limited information.
References	Smith CC (1953). Toxicity of butyl stearate, dibutyl sebacate, dibutyl phthalate and methoxyethyl oleate,. AMA Arch. Ind. Occup. Med. **7:** 310-318.
Other	Date: November 11, 2003.

Repeated-Dose Toxicity (CAS No. 123-95-5)

Test Substance	Stearic acid, butyl ester
CAS Number	123-95-5
Remarks	Purity not specified
Method/guideline	Not specified
Test type	Two year oral feeding toxicity study
GLP	No
Year	1953
Species/strain	Rats / Sprague Dawley (age 5-6 weeks, weight 65-66 g)
Route of Administ.	Diet containing butyl stearate at 0.01, 0.05, 0.25, 1.25 and 6.25% test material.
Duration of test	Two years
No. of animals	Group of 16 male rats
Dose/Conc. Levels	0, 0.01, 0.05, 0.25, 1.25 and 6.25% in diet
Sex	Male rats (16 /treatment group)
Frequency of treatment	Daily administration in diet
Control Group	Yes, two control groups
Post-exposure observat.	Mortality, survival, growth, food consumption clinical observations, clinical chemistry, hematology, necropsy, gross morphology, and histopathology were carried out.
Statist. Methods	Not specified.
Remarks on Test Conditions	Smith (1953) reported only the results for the animals in the control groups and in the two groups receiving the two highest doses (1.25% and 6.25%). The findings for the other dose groups were reported to be not significantly different. At concentrations of 1.25% and 6.25% in the diet, exposed rats showed no significant differences from control animals with respect to growth, survival, blood counts or other hematological parameters. Other pathological changes such as tumors and infections were found in older rats and were not considered to be treatment-related to butyl stearate. Histopathological changes included chronic pneumonitis, diffuse fatty infiltration in the liver, focal necrosis of hepatic cells surrounding veins and chronic nephrosis but these were observed in both treated and control rats. None of the histopathological changes, however, appeared more frequently among the dosed animals than they did in the control group animals.
Conclusions	NOAEL was estimated to be 6.25% in the diet. The dietary 1.25% and 6.25% concentrations of butyl stearate corresponded approximately to daily doses of ~2500 and 6000 mg/kg/day, respectively.
Data Quality	Reliable with restrictions. [Klimisch reliability 2]. Not GLP.
References	Smith CC (1953). Toxicity of butyl stearate, dibutyl sebacate, dibutyl phthalate and methoxyethyl oleate,. AMA Arch. Ind. Occup. Med. **7:** 310-318. The chronic feeding study has been reviewed and similarly summarized by Elder RL (1985) in J. Amer. Coll. Toxicol. **4(5):** 107-146.
Other	Date: November 11, 2003.

Reproductive /Developmental Toxicity (CAS No. 123-95-5)

Test Substance	Stearic acid, butyl ester
CAS Number	123-95-5
Remarks	Purity not specified
Method/guideline	Not specified
Test type	Reproductive/developmental study
GLP	No
Year	1953
Species/strain	Rats / Sprague Dawley (age 5-6 weeks, weight 65-66 g)
Route of Administ.	Diet containing butyl stearate at 6.25% test material.
Duration of test	10 weeks
No. of animals	20 /sex
Dose/Conc. Levels	0 and 6.25% in diet
Sex	Male and female rats (20 per sex)
Frequency of treatment	Daily administration in diet at 6.25% for 10 weeks before mating
Control Group	Yes, 12 male and 12 female in control group
Statist. Methods	Not applicable
Remarks on Test Conditions	Groups of 20 male and 20 female rats were fed diets containing 6.25% of butyl stearate for 10 weeks and then mated. A control group of 12 male and 12 female rats were fed the basal ration for 10 weeks and mated. Females when pregnant were transferred to individual breeding cages and the date of parturition and the number of young in each litter were recorded. Litters were weaned 21 days postpartum and the weights of the weanling determined. From each of the three groups of weanling (those on the test material and the controls), 24 males and 24 females were chosen at random and for the next 21 days, these young were fed the same 6.25% diet as had been ingested by their parents. Diet intake and body weights were recorded daily; 21 days after weaning, the rats were sacrificed and necropsies were performed.
Results/Remarks	Smith (1953) concluded that ingestion of a diet containing 6.25% butyl stearate had no adverse effect on fertility, on the size of the litter, or on survival of the offspring. However, at the 6.25% dietary concentration, significant retarded growth during the preweaning and postweaning period were caused by the test material in comparison with the controls. No gross pathologic changes were found among the young rats during necropsy at the end of the 21-day postweaning period.
Conclusions	NOAEL was 6.25% in diet (ca. 6000 mg/kg/day) (based on effect on reproduction, fertility, litter size and survival of offspring).
Data Quality	Reliable with restrictions. [Klimisch reliability 2]. Not GLP.
References	Smith CC (1953). Toxicity of butyl stearate, dibutyl sebacate, dibutyl phthalate and methoxyethyl oleate,. AMA Arch. Ind. Occup. Med. **7:** 310-318. The chronic feeding study has been reviewed and similarly summarized by Elder RL (1985) in J. Amer. Coll. Toxicol. **4(5):** 107-146.
Other	Date: November 11, 2003.

Acute Oral Toxicity (CAS No. 85049-37-2)

Test Substance	Fatty acids, C16-18 saturated and C18-unsaturated, 2-ethylhexyl ester
CAS Number	85049-37-2
Remarks	Purity not specified
Method/guideline	Not indicated
Test type	Acute oral toxicity (limit-test)
GLP	No
Year	1971
Test system	Species (Strain) Rat (not specified) Sex: Not specified No. of animals: Not specified Route: Oral gavage Dosage: 20 ml/kg body weight or 17.2 g/kg (based on density of 0.86 g/ml for test material)
Test conditions	Remarks: Test material was administered by oral gavage to rats at 20 ml/kg (equivalent to 17.2 g/kg)
Results/Remarks	Acute oral toxicity study (unpublished proprietary study) was cited as having been carried out with substance having CAS No. 85049-37-2.
Conclusions	The acute oral LD_{50} was > 17.2 g/kg.
Data Quality	Not assignable [Klimisch reliability 4]. Limited experimental information as reported in IUCLID (1996).
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Fatty Acids, C16-18 and C18-unsatd, 2-Ethylhexyl Esters, CAS No. 85049-37-2. 23 pages. October 26, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 13, 2003.

Genetic Toxicity In vitro (CAS No. 85049-37-2)

Test Substance	Fatty acids, C16-18 saturated and C18-unsaturated, 2-ethylhexyl ester
CAS Number	85049-37-2
Remarks	Purity not specified
Method/guideline	Not specified
Type of Study	Ames *Salmonella* Mutation Assay
Test System	Bacterial
GLP	No
Year	1988
Species/Strain	*Salmonella typhimurium* / TA98, TA100, TA1535, TA 1537, TA 1538
Metab. Activation	Yes. Metabolic activation system used in Ames assay but specific information not given.
Concentrations	8,40, 200, 100 and 5000 µg/plate.
Statist. Methods	Not specified
Remarks on Test Conditions	Limited experimental information given but study presumably followed Ames assay procedures, with and without metabolic activation.

Conclusions	The test substance was negative in the *Salmonella typhimurium* reverse mutation assay, with and without metabolic activation. IUCLID (1996) noted that genotoxicity data assessment for CAS No. 85049-37-2 was based on test data for mixture of isooctylpalmitate and isooctylstearate.
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature. Limited information and experimental details. Mutagenicity assessment of test material was based on test results for structurally analogous material, namely, mixture of isooctylpalmitate and isooctylstearate.
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Fatty Acids, C16-18 and C18-unsatd, 2-Ethylhexyl Esters, CAS No. 85049-37-2. 23 pages. October 26, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 13, 2003.

Acute fish toxicity (CAS No. 85049-37-2)

Test Substance	Fatty acids, C16-18 saturated and C18-unsaturated, 2-ethylhexyl ester
CAS Number	85049-37-2
Remarks	Purity not specified
Method/guideline	ISO 7346/1-3 Semi-static test version (ISO 7346/2)
Type (test type)	96-hr Acute Fish Toxicity
Test System	Fish, freshwater
GLP	Not specified
Year	1984
Species/Strain	Fish: Brachydanio rerio
Analyt. Monitoring	Not indicated.
Exposure period	96 hours
Statist. Methods	Not specified
Remarks on Test Conditions	Limited experimental information given. Test material was a poorly water-soluble substance that was directly weighed into test vessel followed by treatment with Ultraturrax for 10 minutes before water mixture or WAF was tested.
Result/Conclusion	96-hr LC50 was reported to be 3200 mg/L as cited in IUCLID dataset (1996). The data would indicate that the test substance did not cause mortality in fish at or close to its water saturation levels or water solubility limits (WSL).
Data Quality	Not assignable [Klimisch reliability 4]. Cited in IUCLID dataset for CAS No. 85049-37-2
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Fatty Acids, C16-18 and C18-unsatd, 2-Ethylhexyl Esters, CAS No. 85049-37-2. 23 pages. October 26, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 13, 2003.

Acute toxicity to aquatic invertebrate (CAS No. 85049-37-2)

Test Substance	Fatty acids, C16-18 saturated and C18-unsaturated, 2-ethylhexyl ester
CAS Number	85049-37-2
Remarks	Purity not specified
Method/guideline	Method conforms with OECD 202 guidelines
Type (test type)	Daphnia sp. Acute immobilization test .
Test System	Freshwater invertebrate
GLP	Not specified
Year	Not specified
Species/Strain	Freshwater invertebrate, *Daphnia magna*
Analyt. Monitoring	Not indicated
Exposure period	24 hours
Statist. Methods	Not specified
Remarks on Test Conditions	Limited experimental information given. Test material was a poorly water-soluble substance that was directly weighed into test vessel followed by treatment with Ultraturrax for 10 minutes and ultrasound for 5 minutes before water mixture or WAF was tested.
Result/Conclusion	24-hr EC_{50} was reported to be 17 mg/L as cited in IUCLID dataset (1996) EC_0 was cited as 3 mg/L. The data would suggest that test substance did not cause immobilization at or close to its water saturation levels or water solubility limits (WSL).
Data Quality	Not assignable [Klimisch reliability 4]. Cited in IUCLID dataset for CAS No. 85049-37-2
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Fatty Acids, C16-18 and C18-unsatd, 2-Ethylhexyl Esters, CAS No. 85049-37-2. 23 pages. October 26, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 13, 2003.

Acute toxicity to aquatic plants (e.g., algae) (CAS No. 85049-37-2)

Test Substance	Fatty acids, C16-18 saturated and C18-unsaturated, 2-ethylhexyl ester
CAS Number	85049-37-2
Remarks	Purity not specified
Method/guideline	Method reported to conform to OECD 201 guidelines
Type (test type)	Algae, growth inhibition test
Test System	Aquatic plant (e.g., algae)
GLP	Not indicated
Year	Not specified
Species/Strain	Algae (*Scenedesmus subspicatus)*
Analyt. Monitoring	Not indicated
Exposure period	96 hours
Statist. Methods	Not specified
Remarks on Test Conditions	Limited experimental information given. Biomass was toxicity endpoint monitored for algae growth or inhibition. Test material was a poorly water-soluble substance that was directly weighed into test vessel followed by treatment with ultrasound for 5 minutes before water mixture or WAF was tested.

Results/ Conclusions	96-hr EC_{50} was reported to be 40-42 mg/L as cited in IUCLID dataset (1996) EC_{10} was cited as 17-18 mg/L. Data would suggest that test substance did not cause algae growth inhibition at or close to its water saturation levels or water solubility limits (WSL).
Data Quality	Not assignable [Klimisch reliability 4]. Cited in IUCLID dataset for CAS No. 85049-37-2
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Fatty Acids, C16-18 and C18-unsatd, 2-Ethylhexyl Esters, CAS No. 85049-37-2. 23 pages. October 26, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 13, 2003.

Biodegradation (CAS No. 85049-37-2)

Test Substance	Fatty acids, C16-18 saturated and C18-unsaturated, 2-ethylhexyl ester
CAS Number	85049-37-2
Remarks	Purity not specified
Method/guideline	OECD 301D Closed Bottle Test
Test type	Aerobic Ready Biodegradability test
GLP	Yes
Year	1991
Test system	Exposure Period: 28 Days Inoculum: Activated sludge Kinetics: Not Reported Monitoring: Biochemical oxygen demand, oxygen uptake
Test Conditions	Limited experimental information on aerobic biodegradation study was given.
Results/ Conclusions	Biodegradation was reported to be 85% in 28 days. Information regarding positive controls and blanks was not reported. No data given on whether test material met readily biodegradable classification.
Data Quality	Not assignable [Klimisch reliability 4]. Cited in IUCLID dataset for CAS No. 85049-37-2
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Fatty Acids, C16-18 and C18-unsatd, 2-Ethylhexyl Esters, CAS No. 85049-37-2. 23 pages. October 26, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 13, 2003

Acute Oral Toxicity (CAS No. 109-36-4)

Test Substance	Stearic acid, octyl ester
CAS Number	109-36-4
Remarks	Purity not specified
Method/guideline	Not indicated
Test type	Acute oral toxicity

GLP	No
Year	1985
Test system	Species (Strain) Rat (not specified) Sex: Male and female No. of animals: 5/sex/treatment Route: Oral gavage, undiluted Dosage: 8 ml/kg body weight
Test conditions	Remarks: Test material was administered by oral gavage to 5 female and 5 male rats at 8 ml/kg. Mortality, clinical signs and body weight gain were monitored during 14-day period. Statistical methods were not specified.
Results/Remarks	Elder (1985) reported that no deaths in the dosed animals during the 14-day observation period. Body weight gain of test animals during the 2 weeks averaged 25.7%. The investigators considered acute toxicity of test material to be "very low".
Conclusions	The acute oral LD_{50} > 8 ml/kg.
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature. Limited experimental information
References	Elder RL (1985). Final report on the safety assessment of butyl stearate, cetyl stearate, isobutyl stearate, isopropyl stearate, myristyl stearate and octyl stearate , J. Amer. Coll. Toxicol. 4(5): 107-146.
Other	Date: November 12, 2003.

Repeated-Dose Toxicity (CAS No. 109-36-4)

Test Substance	Stearic acid, octyl ester
CAS Number	109-36-4
Remarks	Purity not specified
Method/guideline	Not specified
Test type	28-Day Oral Toxicity Study
GLP	Yes
Year	1991
Species/strain	Rats /Sprague Dawley
Route of Administ.	Oral gavage
Duration of test	28 days
No. of animals	Not specified
Dose/Conc. Levels	0, 100, 500 and 1000 mg/kg body weight
Sex	Male and female
Frequency of treatment	Oral gavage, 1/day, 5 days/week for 28 days
Control Group	Yes
Post-exposure observat.	Mortality, clinical and biochemical parameters, histopathology,
Statist. Methods	Not specified.
Remarks on Test Conditions	Aulmann et al. (2003) and IUCLID (1996) have reported that a 28-day oral toxicity study in which rats were dosed with up to 1000 mg/kg of the substance, which was octyl stearate (2-ethylhexylstearate). It was reported that 28-day oral exposure to 1000 mg/kg doses did not alter any clinical or biochemical parameters. In addition, other in-life parameters, macroscopic and microscopic (histopathological) examination of

Conclusions	the organs revealed no treatment-related effects, even at the highest dose of 1000 mg/kg. IUCLID (1996) reported that the NOAEL was 1000 mg/kg. Oral gavage of the test substance to rats at dose levels up to 1000 mg/kg/day over 28 days resulted in no systemic toxicity and no histopathological observations that were treatment-related.
Data Quality	Reliable with restrictions [Klimisch reliability 2]. This 28-day repeated dose study was reported as unpublished proprietary data in IUCLID dataset and cited by Aulmann et al. (2000)
References	1) Aulmann W, Pittermann W, Bartnik F, Sterzel W, Kastner W, Potokar (2000). Developmental toxicity of 2-ethylhexyl stearate. Food Chem. Toxicol. **38:** 57-63. 2) IUCLID (1996). ECB Existing Chemicals Datasheet for Fatty Acids, C16-18, 2-Ethylhexyl Esters, CAS No. 91031-48-0. 14 pages. October 26, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 13, 2003.

Genetic Toxicity In Vitro (CAS No. 109-36-4)

Test Substance	Stearic acid, octyl ester
CAS Number	109-36-4
Remarks	Purity was not indicated
Method/guideline	Not specified
Type of Study	Ames *Salmonella* Mutation Assay
Test System	Bacterial
GLP	No
Year	Not specified
Species/Strain	*Salmonella typhimurium* / Tester strains not specified
Metab. Activation	Yes. Metabolic activation system used in Ames assay but specific information not given.
Concentrations	Highest dose concentration was reported to be 5000 μg/plate.
Statist. Methods	Not specified
Remarks on Test Conditions	Limited experimental information given but Ames assay was performed with and without metabolic activation.
Conclusions	The test substance was negative in the *Salmonella typhimurium* reverse mutation assay, with and without metabolic activation.
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature. Limited information and experimental details. Mutagenicity data was cited by Aulmann et al. (2000) in summary review of toxicity data for 2-ethylhexyl stearate.
References	Aulmann W, Pittermann W, Bartnik F, Sterzel W, Kastner W, Potokar (2000). Developmental toxicity of 2-ethylhexyl stearate. Food Chem. Toxicol. **38:** 57-63.
Other	Date: November 13, 2003.

Developmental Toxicity (CAS No. 109-36-4)

Test Substance	Stearic acid, octyl ester
CAS Number	109-36-4
Remarks	Purity was not indicated
Method/guideline	OECD 414
Test type	Developmental toxicity study
GLP	Yes
Year	2000
Species/strain	Rat / Sprague Dawley CD, 8 weeks old, mean body weight 197 g
Route of Administ.	Oral gavage in vehicle (arachidis oil)
Duration of test	20 days
Sex, No. of animals	24 mated females/treatment
Dose/Conc. Levels	0 (arachidis oil), 100, 300 and 1000 mg/kg body weight
Frequency of treatment	Daily from Gestation Day 6-15, inclusive
Control Group	Yes, untreated controls (vehicle: arachidis oil)
Statist. Methods	Dunnett test, Steel test, Fischer's exact test for 2x2 tables
Remarks on Test Conditions	Mated female rats were orally gavaged daily on gestation day 6 up to day 15 post coitum (pc). Observations: mortality and clinical signs of dams were noted daily from day 0 to 20. Body weight was recorded on day 0, 6, 16 and 20. Body weight gains were calculated based on body wt on day 0 of gestation. All females were sacrificed and subjected to macroscopic examination of all maternal organs on day 20. The uteri were removed, weighed and examined for number of corpora lutea, number of implantation sites and number and location of fetuses and resorptions. Fetuses were inspected on total number, sex, weight, external and visceral defects (½ of fetuses by the modified Wilson technique and ½ of fetuses were cleaned in potassium hydroxide and stained with Alizarin red by Dawson's technique). Visceral examination was performed and alterations of fetuses classified into four categories: variations, retardations, anomalies and malformations.
Results	Maternal data: Test material did not affect maternal rats during the entire pregnancy. No mortalites occurred in the dams during the study either in vehicle controls or in the group exposed to test material up to 1000 mg/kg bw. The absolute and corrected b.w. and b.w. gains were comparable between the groups. Gross macroscopic examination of the maternal organs including ovaries and uterus revealed no alterations or gross lesions. Dams tolerated all dose levels without any toxic effects. The NOAEL of 1000 mg/kg for maternal toxicity. Fetal data: All females had viable fetuses. Pre- and post-implantation loss and mean numbers were not affected by treatment. All parameters were comparable with the animals of the control group. Skeletal and visceral investigations detected no treatment-related malformations. For the embryo/fetotoxicity and teratogenicity, the NOAEL was 1000 mg/kg b.w.
Conclusions	NOAEL was 1000 mg/kg for embryo-/fetotoxicity, teratogenicity and maternal toxicity There were no treatment-related effects on developmental toxicity parameters.
Data Quality	Reliable without restrictions [Klimisch reliability 1]. Study was conducted in compliance with OECD 414 guideline and GLP.
References	Aulmann W, Pittermann W, Bartnik F, Sterzel W, Kastner W, Potokar (2000). Developmental toxicity of 2-ethylhexyl stearate. Food Chem. Toxicol. **38:** 57-63.
Other	Date: November 13, 2003.

Acute Oral Toxicity (CAS No. 3687-46-5)

Test Substance	Oleic acid, decyl ester
CAS Number	3687-46-5
Remarks	Purity not specified
Method/guideline	Not indicated
Test type	Acute oral toxicity
GLP	No
Year	1982
Test system	Species (Strain) Rat (Wistar) Sex: Male and female No. of animals: 3 Males and 2 Females/treatment dose Route: Oral Gavage Dosage: 2.5, 5.0, 10.0, 20.0 and 40.0 ml/kg
Test conditions	Remarks: Test material was administered by oral gavage to group of 5 rats (three male and two female) per dose level. The animals were fasted for 24 hrs prior to dosing. Animals were observed for mortality and clinical signs daily for 14-day period. Statistical methods were not specified.
Results/Remarks	Elder (1982) reported no deaths in any of the dosed animals. The LD_{50} was estimated to be > 40 ml/kg body weight.
Conclusions	The acute oral LD_{50} > 40 ml/kg b.w.
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature. Limited experimental information
References	Elder RL (1982). Final report on the safety assessment of decyl and isodecyl oleates. J. Amer. Coll. Toxicol. 1(2): 85-95.
Other	Date: November 12, 2003.

Repeated-Dose Toxicity (CAS No. 3687-46-5)

Test Substance	Oleic acid, decyl ester
CAS Number	3687-46-5
Remarks	Purity not specified
Method/guideline	OECD 407 Repeated 28 day Oral Toxicity
Test type	28-Day Oral Toxicity Study
GLP	No
Year	1987
Species/strain	Rats / Wistar Han
Route of Administ.	Oral gavage
Duration of test	28 days
No. of animals	Information not reported
Dose/Conc. Levels	0, 100, 500, and 1000 mg/kg/day
Sex	Male and female
Frequency of treatment	Daily oral gavage, 5 times per week for 28 days
Control Group	Yes

Post-exposure observat.	There were post-exposure observations and it appears that mortality, clinical signs, clinical chemistry, hematology, gross morphology, necropsy were performed.
Statist. Methods	Not specified.
Remarks on Test Conditions	The test substance was administered by oral gavage daily, 5 times per week for four weeks to Wistar rats at dose levels of 0, 100, 500 and 1000 mg/kg body weight. Oral (gavage) administration of the test substance to male and female Wistar rats at dose levels up to 1000 mg/kg/day for 28 days, produced no systemic toxicity. No deaths were cited. Also, IUCLID reported that even at the highest dose, no substance-related effects were noted with respect to clinical symptoms, biochemistry, hematology, gross lesions and histopatholological evidence of organ injury.
Conclusions	1) NOAEL was 1000 mg/kg/day. 2) Oral gavage of the test substance to Wistar rats at dose levels up to 1000 mg/kg/day over 28 days resulted in no systemic toxicity or adverse toxicity findings. 3) There was no mention of histopathological or gross abnormalities associated with the male or female reproductive organs. .
Data Quality	Reliable with restrictions [Klimisch reliability 2]. This 28-day repeated dose study was reported as unpublished proprietary data in the 1996 IUCLID document. Not GLP.
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Decyl Oleate, CAS No. 3687-46-5. 24 pages. October 23, 1995. Information from IUCLID CD-ROM (version 1996).
Other	Date: November 12, 2003.

Genetic Toxicity In vitro (CAS No. 3687-46-5)

Test Substance	Oleic acid, decyl ester
CAS Number	3687-46-5
Remarks	Purity not specified
Method/guideline	Not specified
Type of Study	Ames *Salmonella* Mutation Assay
Test System	Bacterial
GLP	No
Year	1979
Species/Strain	*Salmonella typhimurium* /TA98; TA100; TA1535; TA1537; TA1538
Metab. Activation	Yes. Metabolic activation system used in Ames assay but specific information not given.
Concentrations	Range from 4 to 2500 μg/plate.
Statist. Methods	Not specified
Remarks on Test Conditions	Limited experimental information given but Ames assay was performed with and without metabolic activation.
Conclusions	The test substance was negative in the strains tested. No mutagenic activity was reported over a dose range from 4 to 2500 μg/plate, with or without metabolic activation.
Data Quality	Reliable with restrictions [Klimisch reliability 2]. Not GLP and based on unpublished proprietary information as cited in IUCLID dataset.
References	IUCLID (1996). ECB Existing Chemicals Datasheet for Decyl Oleate, CAS No. 3687-46-5. 24 pages. October 23, 1995. Information from IUCLID CD-ROM (version 1996)
Other	Date: November 12, 2003.

Melting Point (CAS No. 17661-50-6)

Test Substance **CAS Number** **Remarks**	Stearic acid, myristyl ester 17661-50-6 Purity not specified
Method/guideline	Not specified.
Test type **GLP** **Year**	Melting point Not specified No specified
Remarks	Method of melting point determination was not given.
Conclusions	Melting Point: 54 °C Citation by Syracuse Research Corp. This m.p. value was reported actual value in the exptl melting point database under CAS No. 17661-50-6.
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature.
References	Syracuse Research Corp. This value was cited for melting point for test material under CAS No. 17661-50-6 in EpiWin experimental database as printed out in Epi summary report.
Other	Date: November 10, 2003.

Acute Oral Toxicity (CAS No. 17661-50-6)

Test Substance **CAS Number** **Remarks**	Stearic acid, myristyl ester 17661-50-6 Purity not specified
Method/guideline **Test type** **GLP** **Year**	Not indicated Acute oral toxicity No 1985
Test system	Species (Strain) CFW Mice (Carworth) Sex: Not specified No. of animals: 20/treatment Route: Oral gavage
Test conditions	Remarks: Test material was administered by oral gavage to CFW mice (20 mice) at 10 g/kg. Mortality observed over 5 day period. Statistical methods were not specified.
Results/Remarks	Elder (1985) reported that no deaths or visible "untoward effects"were observed in mice. The LD_{50} was estimated to be > 10 g/kg body weight.
Conclusions	The acute oral LD_{50} > 10 g/kg in mice.
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature. Limited experimental information
References	Elder RL (1985). Final report on the safety assessment of butyl stearate, cetyl stearate, isobutyl stearate, isopropyl stearate, myristyl stearate and octyl stearate , J. Amer. Coll. Toxicol. 4(5): 107-146.
Other	Date: November 11, 2003.

Acute Oral Toxicity (CAS No. 25339-09-7)

Test Substance **CAS Number** **Remarks**	Stearic acid, isocetyl ester 25339-09-7 Purity not specified
Method/guideline **Test type** **GLP** **Year**	Not indicated Acute oral toxicity No 1985
Test system	Species (Strain) Rats (not specified) Sex: Not specified No. of animals: 10/treatment Route: Oral gavage
Test conditions	Remarks: Test material was administered by oral gavage at 10 g/kg, undiluted, to a group of 10 rats. Mortality was observed over 72-hr period. Statistical methods were not specified.
Results/Remarks	Elder (1985) reported that no deaths occurred and the test material was considered by the investigators of the study to be non-toxic. The LD_{50} was estimated to be > 10 g/kg body weight.
Conclusions	The acute oral LD_{50} for the test substance was reported to be > 10 g/kg .
Data Quality	Not assignable [Klimisch reliability 4]. Secondary literature. Limited experimental information.
References	Elder RL (1985). Final report on the safety assessment of butyl stearate, cetyl stearate, isobutyl stearate, isopropyl stearate, myristyl stearate and octyl stearate , J. Amer. Coll. Toxicol. 4(5): 107-146.
Other	Date: November 11, 2003.