CAS# 61788-44-1
Styrenated Phenol

Molecular Weight: **322 (Typical)**

1.1 GENERAL SUBSTANCE INFORMATION

A.	**Type of Substance:**	Organic
B.	**Physical State:**	Clear pale yellow to amber liquid
C.	**Purity:**	98-99+ % Typical for Commercial Products

1.2 SYNONYMS

Wingstay® S
Montaclere® S
Montaclere® SE
Kumanox® SP
Vulcanox® SP
Vanox® 102
Naugard® SP
SP
SPH

1.3 IMPURITIES Phenol (108-95-1) < 1%

1.4 ADDITIVES None

2. PHYSICAL-CHEMICAL DATA

***2.1 MELTING POINT**

Value:	<0°C
Decomposition:	No
Sublimation:	No
Method:	None
GLP:	No data
Remarks:	Liquid at 0°C
Reference:	Flexsys America L.P.

***2.2 BOILING POINT**

Value:	230 °C
Pressure:	1013 hPa
Decomposition:	No
Method:	Not Determined
GLP:	No data
Remarks:	None
Reference:	Monsanto Toxicology Profile – Montaclere, November 15, 1988
Reliability:	(2) Valid with restrictions – no detail

†2.3 DENSITY

Type:	Density
Value:	1.08
Temperature:	20°C
Method:	Flexsys Standard Method of Analysis FF97.4-1
GLP:	Yes
Remarks:	Hydrometer method. Hydrometer must meet standards set in ASTM-E-100
Reference:	ASTM D891-94 method equivalent
Reliability:	(1) Valid without restriction

***2.4 VAPOUR PRESSURE**

Value:	0.04413 hPa (0.0331 mm Hg)
Temperature:	25 °C
Method:	calculated Other: Modified Grain method
GLP:	No
Remarks:	Estimation method based on molecular structure and measured Boiling point of 230°C
Reference:	EPIWIN/MPBPWIN v1.40
Reliability:	(2) Valid with restrictions – Modelling data

***2.5 PARTITION COEFFICIENT $\log_{10}P_{ow}$**

Log Pow:	2.41
Temperature:	Not Applicable
Method:	calculated SRC LogKow (KowWin) Program, 1995
GLP:	No
Remarks:	Accepted calculation model using molecular structure and measured boiling point of 230°C
Reference:	Meylan, W.M. and. P.H. Howard, 1995 J. Pharm. Sci. 84: 83-92
Reliability:	(2) Valid with restrictions – modelling data

log Pow:	> 4 at 22 degree C
Method:	other (measured)
Year:	
GLP:	no
Reference:	(20)
Reliability:	(2) valid with restrictions

***2.6 WATER SOLUBILITY**

A. Solubility

B. pH Value

pH Value:	6.9-7.2.
Concentration:	1% Emulsion
Temperature:	25 °C
Method:	Flexsys Standard Method of Analysis FF83.11-1.
GLP:	Yes
Remarks:	Potentiometric measurement
Reference:	JIS K6220 Product Specification Test Method
Reliability:	(1) Valid without restriction

Value:	59 mg/l at 20 degree C
pH:	5.6 - 5.9
Method:	other
GLP:	yes
Reference:	(20)
Reliability:	(1) valid without restriction

2.7 FLASH POINT (Liquids)

Value:	>180°C
Type:	Cleveland Open Cup
Method:	ASTM D 92-96
Year:	1996
GLP:	Yes
Remarks:	Standard Test Method for Flash and Fire Points by Cleveland Open Cup
Reference:	Kumho Monsanto Inc. QA/QC Laboratory, 2002
Reliability:	(1) Valid without restriction

†2.12 OXIDATION: REDUCTION POTENTIAL

2.13 ADDITIONAL DATA

A. Partition co-efficient between soil/sediment and water (Kd)

B. Other data – Henry's Law Constant

Results:	1.58E-006 atm-m3/mole
Remarks:	Calculated at 25°C using measured boiling point of 230°C
Reference:	Environ Toxicol Chem 10: 1283-93 (1991) EPIWIN/HENRYWIN v3.10
Reliability:	(2) Valid with restrictions – Modelling data

3. <u>ENVIRONMENTAL FATE AND PATHWAYS</u>

***3.1.1 PHOTODEGRADATION**

Type:	air
INDIRECT PHOTOLYSIS	
Sensitizer:	OH
Conc. of sens.	1560000 molecule/cm3
Rate constant:	57.7729E-12 cm3/(molecule-sec)
Degradation:	50 % after 2.222 hours
Method:	other (calculated): AOP Program (v1.89)
Year:	1999
GLP:	No
Test substance:	other TS: molecular structure and measured boiling point of 230°C
Reference:	EPIWIN/AOPWIN v1.90
Reliability:	(2) Valid with restrictions - Accepted calculation method

***3.1.2 STABILITY IN WATER**

***3.2 MONITORING DATA (ENVIRONMENTAL)**

3.3 TRANSPORT AND DISTRIBUTION BETWEEN ENVIRONMENTAL COMPARTMENTS INCLUDING ESTIMATED ENVIRONMENTAL CONCENTRATIONS AND DISTRIBUTION

***3.3.1 TRANSPORT**

Type:	Adsorption
Media:	Soil/Sediment
Method:	SRC Structure estimation method based on molecular connectivity indices, 1992
Results:	Koc =856.1; Log Koc = 2.933
Remarks:	Estimation based on molecular structure and measured boiling point of 230°C
Reference:	EPIWIN/PCKOCWIN v1.66
Reliability:	(2) Valid with restrictions – Modelling data

Type:	Volatility
Media:	Water
Method:	Estimation Method, 1990
Results:	Volatilization half-life from model river: 1856 hours Volatilization half-life from model lake: 2.034E+004 hours
Remarks:	Model river = 1 m deep flowing at 1 m/sec and wind velocity of 3 m/sec. Model lake = 1 m deep flowing at 0.05 m/sec and wind velocity of 0.5 m/sec.
Reference:	Handbook of Chemical Property Estimation Methods, 1990
Reliability:	(2) Valid with restrictions – Peer-reviewed published data from a generally accepted and validated estimation method

***3.3.2 THEORETICAL DISTRIBUTION (FUGACITY CALCULATION)**

Media:	Air-biota-sediment-soil-water			
Method:	Fugacity level III EPIWIN v3.10			
Results:		Mass Amount (%)	Half-life (hrs)	Emissions (kg/hr)
	Air	00.51	3.32	1000
	Water	41.10	360	1000
	Soil	58.20	360	1000
	Sediment	00.194	360	0
Remarks:	Persistence time = 291 hours Calculation based on molecular structure and measured boiling point of 230°C			
Reference:	EPISUITE/EPIWIN v3.10			
Reliability:	(2) Valid with restrictions – Modelling data			

***3.5 BIODEGRADATION**

Type:	aerobic
Inoculum:	activated sludge
Degradation:	7 % after 28 day Method: other: OECD 301 Manometric Respirometry modified according to EEC Round Robin Test "Assessment of Biodegradability of Chemicals in Water by anometric Respirometry" DGX 1/283/82 Rev 5, EEC 79/831, Annex 5, Part C
Year:	1990 GLP: yes
Test substance:	Styrenated phenol
Reference:	(21)
Reliability:	(1) valid without restriction

3.6 BIOACCUMULATION

Species:	Other
BCF:	14.43
Method:	BCFWIN v2.14
GLP:	No
Remarks:	Calculated using molecular structure and measured boiling point of 230°C. Log BCF = 1.159
Reference:	EPIWIN/BCFWIN v2.14
Relaibility:	(2) Valid with restrictions – modelling data

4. ECOTOXICITY

*4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type:	static
Species:	Brachydanio rerio (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: yes
LC0:	1
LC100:	10
Geom. mean: :	3.2
Method:	other: UBA-Verfahrensvorschlag "Letale Wirkung beim Zebrabaerbling Brachydanio rerio" (LC0, LC 50, LC100: 48-96 Studen) (May, 1984)
Year: 1991	GLP: yes
Test substance:	other TS: 99.97%
Remark:	Nominal concentrations; to produce the test solutions, the substance was weighed into water and homogenized in an Ultra-Turrax unit for 60 seconds at 8000 r.p.m. Undissolved particles (oily droplets) of the substance remained on the surface of the test medium at all test concentrations (10 mg/l turbid emulsion).
Reference:	(21)
Reliability:	(1) valid without restriction

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

*4.3 TOXICITY TO AQUATIC PLANTS, e.g. algae

4.4 TOXICITY TO MICROORGANISMS e.g. bacteria

Type:	aquatic
Species:	activated sludge
Exposure period:	3 hour(s)
Unit:	mg/l Analytical monitoring: no
EC50:	362
Method:	ISO 8192 "Test for inhibition of oxygen consumption by activated sludge"
Year:	1990 GLP: yes
Test substance:	other TS: 99.97%
Reference:	(21)
Reliability:	(1) valid without restriction

5. TOXICITY

*5.1 ACUTE TOXICITY

5.1.1 ACUTE ORAL TOXICITY

Type:	LD_{50}
Species/strain:	Rats, Sprague-Dawley Albino
Value:	3700 mg/kg bw
Sex:	Male and female
# of Animals:	20
Vehicle:	None - undiluted
Doses:	2510, 3160, 3980 or 5010 mg/kg bw
Method:	Single Oral Dose, Younger Laboratories Protocol, 1973
GLP:	No data
Test substance:	As prescribed by 1.1-1.4, purity: 98%
Remarks:	The test material was administered by gavage to four groups of male and female rats (5 animals/dose level) as an undiluted liquid. Male rats had initial body weights of 230-245 grams: females had initial body weights of 230-245 grams. Clinical signs of toxicity included reduced appetite and activity (two to three days in survivors), followed by increasing weakness, diarrhea, collapse and death. There were no deaths at the two lower dose levels. Gross autopsy findings were that all viscera appeared normal in all survivors; lung hyperemia, slight liver discoloration and gastrointestinal inflammation were noted in the decedents. 95% confidence limits 3400-4000 mg/kg. Statistical calculation of the LD50 was done according to the method of de Beer.

Dose mg/kg	Mortalities-Male	Mortalities-Female	Combined
2510	0/3	0/2	0/5
3160	0/2	0/3	0/5
3980	3/3	1/2	4/5
5010	2/2	3/3	5/5

Reference:	Monsanto Y-75-78 Younger Laboratories May 7, 1975
Reliability:	(2) Valid with restrictions – age of study, lack of method detail

5.1.2 ACUTE INHALATION TOXICITY

Type:	LC_{50}
Species/strain:	Rats, Sprague-Dawley Albino
Sex:	Male
# of Animals:	6
Exposure time:	6 Hours
Value:	> 2.5 mg/L (No mortalities)
Method:	Acute Inhalation LC50, Younger Laboratories Protocol, A.T.S. 1973
GLP:	No data
Test substance:	As prescribed by 1.1-1.4, purity: 98%

Remarks:	Six male rats were exposed to the test substance for six hours at a concentration of 2.5 mg/l in air at 27°C. The concentration was determined by difference between the initial sample weight (133.1g) and the recovered sample weight at the end of the test (129.5g) Airflow rate was 4.0 l/min, chamber volume was 35 l, and humidity was maintained at 80%. No toxic signs of exposure were observed. All animals survived. After a 14-day recovery period, all rats were sacrificed. Gross autopsy results indicated that all viscera appeared normal.
Reference:	Monsanto Y-75-78 Younger Laboratories May 7, 1975
Reliability:	(2) Valid with restrictions – age of study, lack of method detail

5.1.3 ACUTE DERMAL TOXICITY

Type:	LD_{50}
Species/strain:	Rabbits, New Zealand Albino
Value:	>5010 mg/kg bw
Sex:	Male and female
# of Animals:	3
Vehicle:	none
Doses:	5010 or 7940 mg/kg bw
Exposure Time:	24 Hours
Method:	Single Dermal Dose, Younger Laboratories Protocol, 1973
GLP:	No data
Test substance:	As prescribed by 1.1-1.4, purity: 98%
Remarks:	The undiluted test substance was applied to the shaved skin of two groups of male and female rabbits for 24 hours as single dermal application at dose levels of 5010 or 7940 mg/kg/body weight. Mean body weight of males was 1.9 kg, and females, 2.2 kg. The test material was held in place by means of an occlusive wrap of latex rubber and secured by bandaging and elastic tape. The occlusive wrap was removed after 24 hours and the excess material was wiped from the test animal. Clinical observations were made three times during the first eight hours after dosing, and twice daily thereafter until sacrifice. Clinical signs of toxicity included reduced appetite and activity (three to seven days in survivors), followed by increasing weakness, collapse and death at twelve days. Survivors were sacrificed after 14 days. Gross autopsy findings on decedents were slight lung congestion, slight liver and kidney discoloration, enlarged gall bladder, and gastrointestinal inflammation. Gross autopsy findings on the survivors were that all viscera appeared normal.

Dose mg/kg	Mortalities-Male	Mortalities-Female	Combined
5010	0/1	----	0/1
7940	1/1	0/1	1/2

Reference:	Monsanto Y-75-78 Younger Laboratories May 7, 1975
Reliability:	(2) Valid with restrictions – age of study, lack of method detail

5.2.1 SKIN IRRITATION/CORROSION

Species/Strain:	Rabbits, New Zealand Albino
Results:	Severe
# of Animals:	6
Vehicle:	None - undiluted
Value:	6.1/8.0
Results:	Irritating
Classification:	Primary Skin Irritant
Exposure Time:	24 Hours
Method:	Draize, J.H., Woodard, G., and Calvery, H.O., 1944
GLP:	No data
Test substance:	As prescribed by 1.1-1.4, purity: >96%
Remarks:	0.5 ml of the undiluted test substance was applied to the shaved dorsal areas of six albino rabbits. The test material was applied to the skin under 1" square gauze patches and held in contact with the skin by means of an occlusive wrap of latex rubber secured by bandaging and elastic tape. The occlusive wrap and gauze patches were removed after 24 hours. Dermal irritation was scored by the Draize Method, and results were recorded 24, 48, 72 and 168 hours after topical application. The Primary Irritation Index was calculated by averaging the mean scores at 24 and 72 hours. The Primary Irritation Index was found to be 6.1 on a scale of 0.0-8.0. A defatting effect was noted, with skin sloughed off in 10-14 days. There was no injury noted in depth.
Reference:	Monsanto Y-75-78 Younger Laboratories May 7, 1975
Reliability:	(2) Valid with restrictions – age of study, lack of method detail

5.2.2 EYE IRRITATION/CORROSION

Species/strain:	Rabbits, New Zealand Albino
# of Animals:	6
Vehicle:	None - undiluted
Value:	15.4/110.0
Results:	Mild Irritation
Classification:	Irritating
Exposure Time:	24 Hours
Method:	Draize, J.H., Woodard, G., and Calvery, H.O., 1944
GLP:	No data
Test substance:	As prescribed in 1.1-1.4, purity: 98%
Remarks:	0.1 ml of the undiluted test substance was applied to one eye of six albino rabbits. The other eye was not treated and served as a control. The cornea, iris and conjuntivea were examined immediately after treatment, and then at intervals of 10 minutes, 1 hour, and then at 24, 48, 72 and 168 hours. The Draize Method was used for scoring eye irritation. Immediate findings were slight discomfort. At 10 minutes, slight erythema and copious discharge were noted. At one hour, there was moderate erythema, slight edema and copious discharge, At 24 hours, areas of barely perceptible corneal dullness were noted. The iris showed sluggish reaction to light in two animals. There was moderate erythema, slight edema, and copious discharge containing a whitish exudate. At 48 hours – 168 hours,

gradual improvement was noted in all animals. After 10 days, all scored zero. The average Draize score for 24, 48 and 72 hours was calculated for each animal and then averaged over the six animals. The average Draize score was 15.4 on a scale from 0-110.

Reference: Monsanto Y-75-78 Younger Laboratories May 7, 1975
Reliability: (2) Valid with restrictions – age of study, lack of method detail

***5.4 REPEATED DOSE TOXICITY**

Species: rat Sex: male/female
Strain: no data
Route of admin.: oral feed
Exposure period: 90 days (12 weeks)
Frequency of treatment: Daily
Post. obs. period:
Doses: 0, 100, 316, 1000, 3160, and 10,000 ppm (Approximately equivalent to 0, 5, 15.8, 50, 158, and 500 mg/kg body weight/day
Control Group: Yes
NOAEL: 50 mg/kg
LOAEL: 158 mg/kg
Method: Thirty rats/sex/test group and 60 rats/sex in the control group were initiated on study. Rats were observed daily and body weights were measured weekly. Food consumption was measured for at least 10 rats/sex/group during the first 12-weeks of the study. At 12 weeks hematology; blood glucose, urea nitrogen and cholesterol; and urinalysis were conducted on 5 rats/sex/group in the treated groups and 10/sex in the control group. Five rats per treated group and 10 per control group were killed and necropsied. Organ weights were determined for liver, kidney, spleen, heart, adrenals, thyroid, and pituitary. These organs were also examined microscopically. Other select organs were preserved for possible future microscopic examination. The remaining test animals were continued on for a possible chronic toxicity study. (See 36-Week Oral Feeding Study) (Protocol complied with "Appraisal of Food and Drug Chemicals in Foods, Drugs, and Cosmetics", Association of Food and Drug Officials of the United States, 1959.
Year: 1961 GLP: no
Test substance: Styrenated phenol

Result: 12–week feeding study in rats was done at doses from 5 to 500 mg/kg/day. At 158 and 500 mg/kg/day, body weights gain were statistically significantly lower than controls. Liver weights relative to body weights were statistically higher than controls. (No absolute organ weight reported.) Minimal focal thyroid hyperplasia was observed at 500 mg/kg/day. No adverse effects were noted in the clinical pathology evaluations. (including coagulation and prothrombin time.)
Reference: (18)
Reliability: (2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment

Species: rat Sex: male/female
Strain: no data
Route of admin.: oral feed
Exposure period: 36 Weeks
Frequency of treatment: Daily
Post. obs. period:
Doses: 0, 100, 316, 1000, 3160, and 10,000 ppm (Approximately equivalent to 0, 5, 15.8, 50, 158, and 500 mg/kg body weight/day)
Control Group: Yes
NOAEL: 158 mg/kg
LOAEL: 500 mg/kg
Method: Twenty-five rats/sex/test group and 50 rats/sex in the control group were continued on study from the 12-week feeding study. Body weights ere reported at 24 and 36 weeks. Termination of the study was authorized by the sponsor at 36 weeks. Organ weights were determined for liver, kidney, spleen, heart, adrenals, thyroid, and pituitary. Microscopic evaluation of tissues was not done.

Year: 1962 GLP: no
Test substance: Styrenated phenol

Result: 36-week feeding study in rats was done at doses from 5 to 500 mg/kg/day. Statistically lower body weights at 158 and 500 mg/kg/day (body weight gain not reported). Report states that growth was depressed only at 500 mg/kg/day. Increased liver and kidney weights relative to body weight (no absolute organ weights reported). No histopathology and clinical pathology examinations were conducted.
Reference: (19)

Reliability: (4) not assignable

***5.5 GENETIC TOXICITY IN VITRO**

A. BACTERIAL TEST

Type: Microbial Mutagenicity Assay
System of testing: Salmonella typhimurium TA-1535, TA-1537, TA-1538, TA-98, TA-100
Concentration: 0.001, 0.01, 0.1, 1.0 and 5.0 microliters/plate
Metabolic activation: With and without
Results:
Cytotoxicity conc: With metabolic activation: 5.0 ul/plate
Without metabolic activation: 1.0 ul/plate
Precipitation conc: None
Genotoxic effects:
With metabolic activation: Negative

	Without metabolic activation: Negative
Method:	Ames Mutagenicity Plate Test (Overlay Method) 1975
GLP:	Yes
Test substance:	As prescribed in 1.1-1.4, purity: 98%
Remarks:	The test compound was evaluated for genetic activity in microbial assays with and without the addition of mammalian metabolic activation preparations. The *Salmonella typhimurium* strains used for this experiment were obtained from Dr. Bruce Ames. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. Chemicals used as positive controls for the non-activation assays were methylnitrosoguanidine (MNNG), 2-nitrofluorene (NF) and quinacrine mustard (QM). Positive control chemicals used for the activation assays were 2-anthramine (ANTH), 2-acetylaminofluorine (AAF) and 8-aminoquinoline (AMQ). Dimethylsulfoxide (DMSO) was used as the solvent and the solvent control. Analysis included Bartlett's test for homogeneity of variance, and comparison of treatments with controls using within-levels pooled variance and a one-sided t-test. Grubbs' test was performed to determine if outliers were present. The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.
Reference:	Monsanto BIO-76-318 Litton Bionetics January 31, 1977
Reliability:	(1) Valid without restriction

Type:	DNA damage and repair assay
System of testing:	E. coli Pol A+ and Pol A1- Liquid Suspension Assay
Concentration:	10, 25, 50, 75, and 100 micrograms/l
Metabolic activation:	without
Result:	positive
Method:	other
Year:	1981 GLP: no
Test substance:	Styrenated phenol
	Remark: A test for the ability of the chemical to damage cellular DNA in the E. coli Pol A1- Liquid Suspension Assay.
Reference	(22)
Reliability:	(2) valid with restrictions. Meets generally accepted scientific standards, well documented and acceptable for assessment.

B. NON-BACTERIAL IN VITRO TEST

Type:	Mitotic Recombination Assay
System of testing:	Saccharomyces cerevisiae. D4
Concentration:	0.001, 0.01, 0.1, 1.0 and 5.0 microliters/plate
Metabolic activation:	With and without

Results:
Cytotoxicity conc: With metabolic activation: 5.0 ul/plate
Without metabolic activation: 1.0 ul/plate
Precipitation conc: None
Genotoxic effects:
With metabolic activation: Negative
Without metabolic activation: Negative
Method: Ames Mutagenicity Plate Test (Overlay Method) 1975
GLP: Yes
Test substance: As prescribed in 1.1-1.4, purity: 98%
Remarks: The test compound was evaluated for genetic activity in assays with and without the addition of mammalian metabolic activation preparations. The activation system used was S-9 homogenate from Aroclor 1254-induced adult male Sprague-Dawley rat livers. The metabolizing system contained 10% S-9 and cofactors according to the Ames method. The mutagenesis assay was carried out as the plate-incorporation test according to the Ames protocol. The chemical used as the positive control for the non-activation assay was methylnitrosoguanidine (MNNG) at 10 ug/plate. Positive control chemical used for the activation assay was DMNA at 100 micromoles/plate. Dimethylsulfoxide (DMSO) was used as the solvent and the solvent control. Analysis included Bartlett's test for homogeneity of variance, and comparison of treatments with controls using within-levels pooled variance and a one-sided t-test. Grubbs' test was performed to determine if outliers were present. The test compound did not demonstrate mutagenic activity in any of the assays conducted and was considered not mutagenic under the test conditions.
Reference: Monsanto BIO-76-318 Litton Bionetics January 31, 1977
Reliability: (1) Valid without restriction

*** 5.6 GENETIC TOXICITY IN VIVO**

***5.8 TOXICITY TO REPRODUCTION**

***5.9 DEVELOPMENTAL TOXICITY/ TERATOGENICITY**

5.10 OTHER RELEVANT INFORMATION

*** 5.11 EXPERIENCE WITH HUMAN EXPOSURE**

6. REFERENCES

1. Flexsys America L.P. data
2. Monsanto Toxicology Profile – Montaclere, November 15, 1988
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20. Bayer AG, Unpublished Data
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