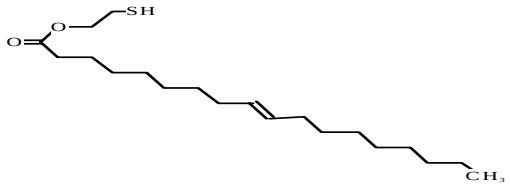
SIDS INITIAL ASSESSMENT PROFILE

CAS No.	68440-24-4
Chemical Name	Fatty acids, tall-oil, 2-mercaptoethyl esters (2-MET)
Structural Formula (and Chemical Identity Information)	2-Mercaptoethyl oleate (representative structure for 2-MET)  Reaction product of tall oil fatty acid with 2-mercaptoethanol (variable) $HSCH_2CH_2OCOC_nH_{2n+1}$ *where n=13 to 17*

SUMMARY CONCLUSIONS OF THE SIAR

Human Health

There were no available data on the toxicokinetic, metabolism or distribution of 2-MET. The oral (gavage) LD_{50} in female rats (1/dose group) of 2-MET is > 800 mg/kg bw but < 2500 mg/kg bw. The LD_{50} in male rats (1/dose group) of 2-MET is > 1700 mg/kg bw but < 2500 mg/kg bw. Instances of nasal discharge, fecal and urinary staining, and/or reduced food consumption; respiration and activity were noted, primarily in the females during the first 24 to 48 hours after dosing. The dermal LD_{50} in rabbits of 2-MET is > 2000 mg/kg bw. Mild to moderate erythema and edema and desquamation were observed. 2-MET is moderately irritating to skin and mildly irritating to the eyes. Sensitisation data are not available for 2-MET.

In a repeated-dose and reproductive/developmental screening study, groups of male and female rats received 2-MET by gavage at doses of 0, 40, 125 and 400 mg/kg bw/d for 14 days prior to mating and during the mating period. Daily dosing of the females was continued throughout pregnancy and up to day 4 of lactation. Males were dosed for at least 46 days and until the day prior to scheduled necropsy. Test item related effects indicative of systemic toxicity were observed in the mid and high dose group. The NOAEL for male animals was 40 mg/kg bw/d based on inflammatory edema of the forestomach; for females the NOAEL was 125 mg/kg bw/d. Repeated-dose inhalation or dermal studies are not available for 2-MET.

An *in vitro* bacterial mutation assay has not revealed any evidence of genotoxic potential of 2-MET. However, an *in vitro* study in mammalian cells (V-79 cells of the Chinese Hamster) with 2-MET was negative for chromosome aberrations in the absence of metabolic activation and equivocal for chromosome aberrations in the presence of metabolic activation. 2-MET was negative in an in vivo mouse micronucleus assay. 2-MET showed evidence for clastogenic potential when tested in vitro.

In the above-mentioned repeated-dose and reproductive/developmental screening study, two high-dose females were found dead on days 20 and 22 of the gestation period, respectively. The cause of death of one female was considered to be test substance-related. The cause of death of the second female could not be established. Beginning near the end of the pre-mating period and until the day before scheduled necropsy, all females in the 400 mg/kg bw/d dose group showed signs of discomfort after administration of the test substance. At 400 mg/kg bw/d, changes in food consumption (males: -5.7%; females: -17.0% pre-pairing, -31.9% lactation) and body weight (-5.7%) were observed in both sexes and mean liver and kidney weights were significantly increased in both sexes. In males, prostate and seminal vesicle weights were significantly decreased. The NOAEL for fertility was 125 mg/kg bw/d based on an increased precoital time, a reduced gestation index and an increase in post-implantation loss at the highest dose tested. The NOAEL for maternal toxicity was 125 mg/kg bw/d based on the above effects at the highest dose. The NOAEL for developmental effects was 40 mg/kg bw/d based on increased liver weight in pups at 125 and 400 mg/kg bw/d. The NOAEL for teratogenicity is 400 mg/kg bw/d (the highest dose tested).

Environment

2-Mercaptoethyl tallate [2-MET] is a mixture produced by a reaction of 2-mercaptoethanol [SCH_3CH_2OH; 2-ME] with tall oil fatty acid [TOFA]. TOFA is a complex mixture of saturated aliphatic straight chain fatty acids made principally of C_{16} but ranging from C_{14} to C_{18} .
The freezing point of 2-MET is 16.9°C and the mean boiling point is 298 °C at 1023.9 hPa. The vapor pressure is 0.00161 hPa at 20 °C. The water solubility of 2-MET is 0.083 mg/L. 2-Mercaptoethyl oleate was used as a representative structure for estimation of partition coefficient and Henry's Law Constant since this oleic acid ester is the predominant component in 2-MET. The estimated log Kow of 2-mercaptoethyl oleate is 8.45 and the Henry's Law Constant is 8.217×10^{-4} atm-m^3/mole. 2-Mercaptoethyl oleate was used as a representative structure for estimation of photodegradation and transport of 2-MET in the environment. The overall OH rate constant for 2-mercaptoethyl oleate ranges from 117.8×10^{-12} cm^3/molecule-sec [cis] to 125.4×10^{-12} cm^3/molecule-sec [trans] with a half-life range in hrs of 1.090 [cis] to 1.024 [trans]. These results apply for photodegradation in air.

The hydrolysis of 2-MET in water without solvent could not be measured due to its very low water solubility (which prevents analysis at extremely low concentrations) and because it is a mixture of fatty acid esters (which makes analyzing the parent compounds and hydrolysis products difficult). However, the hydrolysis of 2-MET was experimentally determined in the presence of co-solvent (50% acetonitrile). Estimated half lives for 2-MET under these conditions at pH 4, 7 and 9 were indefinite, four days and less than one day, respectively. The anticipated hydrolysis products are 2-ME and TOFA. The hydrolysis observed could be more rapid in the presence of acetonitrile than would be observed in the absence of a co-solvent. Therefore, reliably determining the "rate" is problematic because of the limited water solubility.

Level III Fugacity modeling, using loading rates for Air, Soil, and Water of 1000 kg/h for each media, shows the following percent distribution for 2-mercaptoethyl oleate: Air = 0.08%; Soil = 28%; Water = 7.3%; Sediment = 64.6%. In a ready biodegradability test (Modified Sturm Test (CO2 evolution) test), at the end of the 28-day exposure period, the mean biodegradation of the test substance was 71.2%, showing that 2-MET is readily biodegradable. Bioaccumulation is anticipated to be low since the calculated bioconcentration factor of 2-mercaptoethyl oleate is 21.

Aquatic toxicity testing has not been conducted with 2-MET. The aquatic toxicity endpoints have been addressed using surrogate data from the breakdown/hydrolysis products of 2-MET. These breakdown products include 2-mercaptoethanol (2-ME; CAS No. 60-24-2), which was assessed within the OECD HPV Programme and Tall Oil

Fatty Acid (TOFA; CAS No. 61790-12-3), which was assessed in the USEPA HPV Challenge Program.

The following values are available from the short-term tests on aquatic species with 2-ME: fish: LC_{50} (96 h) = 37 mg/l; invertebrates: EC_{50} (48 h) = 0.4 mg/l; algae: E_rC_{50} (72 h) = 18.6 mg/l (E_bC_{50}: 7.0 mg/l). The following values for TOFA are available from the short-term tests on aquatic species with fish, invertebrates and algae: *Pimephales promelas* 96 hr LC50 >1000 mg/L; *Daphnia magna* 48 hr EC50 >1000 mg/L; and *Pseudokirchneriella subcapitata* 72 hr ErC50 >1000 mg/L (72 hr EbC50 = 854.9 mg/L h). Although a chronic daphnia study with 2-MET was proposed, 2-MET has low water solubility, as such a high concentration (50%) of co-solvent is needed to keep 2-MET solubilized, and this level is incompatible with life for any of the aquatic test species. Further, development of a methodology to analyze 2-MET in freshwater to support ecotoxicological studies proved unsuccessful. It appears that several factors potentially including irreversible adsorption to glassware, loss on rotary evaporation and hydrolysis of the ester functionality to the corresponding acid and alcohol precluded the successful development of this methodology.

Exposure

Approximately 12,250 tonnes were produced in the sponsor country (USA) in 2002. Purity of the commercial product ranges from 75 to 95%. Impurities include 0-15 % 2-mercaptoethanol (2-ME; CAS 60-24-2) and 0-15 % tall oil fatty acid (TOFA; CAS 61790-12-3).

In production plants, 2-MET is handled in closed systems (closed piping). Air streams and waste water are treated prior to release to the environment. Air emissions from the manufacturing process are treated using a caustic scrubber and then a thermal oxidizer with a demonstrated removal efficiency > 99.9% for volatile organic compounds (VOCs). Wastewater from the process area is treated on site in a biological wastewater treatment system (primary and secondary treatment). Equipment is not washed with water but instead with solvent or polyvinyl chloride (PVC), which is reprocessed; this method should limit emissions and potential for exposure. Personal protective equipment is used during production to minimize exposure. Worker exposure during manufacture due to non-accidental releases includes exposure during stabilizer sampling and possibly during maintenance. Potential routes of exposure during manufacture include dermal, ingestion and inhalation. 2-MET is stored at ambient temperature in bulk storage tanks with atmospheric vents. This material is transported from the manufacturer by road, marine and air in several container types and sizes.

The predominant uses for 2-MET are as a reactant used in the production of organotin PVC stabilizers and as a diluent in organotin PVC stabilizers. 2-MET's presence within PVC is approved for use as an indirect food additive. Studies showed that 2-MET and other stabilizers did not leach out of the matrix of PVC products.

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health: This chemical is a candidate for further work. The chemicals possess properties indicating a hazard for human health (acute and repeated-dose toxicity, *in vitro* mammalian genotoxicity, and reproductive/developmental toxicity). Member countries are invited to perform an exposure assessment for consumers and workers, and if necessary a risk assessment.

Environment: This chemical is of low priority for further work. The chemical has properties indicating a hazard for the environment (acute toxicity to fish, aquatic invertebrates, and algae (2-ME)). However the chemical is of low priority for further work for the environment because of its rapid biodegradation and its limited potential for bioaccumulation.