MICHIGAN DEPARTMENT OF ENVIRONMENT, GREAT LAKES, AND ENERGY

INTEROFFICE COMMUNICATION

TO: File for Perfluorobutylethylmethyldichlorosilane (CAS # 38436-16-7)

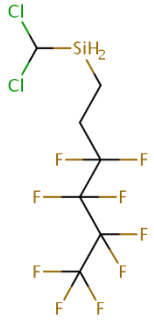
FROM: Brian J. Hughes, Toxics Unit, Air Quality Division

DATE: June 16, 2021

SUBJECT: Screening Level for Perfluorobutylethylmethyldichlorosilane (CAS # 38436-16-7)

Summary
The initial threshold screening level (ITSL) for Perfluorobutylethylmethyldichlorosilane (PFBEMDCS) is 2 µg/m^3 (annual).

Uses and Physical Chemical Properties
PFBEMDCS is manufactured and used as a monomer in polymer production.

Table 1. Physical/Chemical Properties of Perfluorobutylethylmethyldichlorosilane[1]	
Structure	
CAS Number	38436-16-7
Synonyms	Dichloromethyl(3,3,4,4,5,5,6,6,6-nonafluorohexyl)silane
Appearance/Odor	Liquid
Molecular Weight	361.10 g/mol
Melting Point	-42.3 at 20ºC
Boiling Point	164.3℃ at 760 mmHg
Density	1.481 g/cm^3 at 20℃
Vapor Pressure	110 Pa at 20℃ (predicted)
Flash Point	67℃

[1] Information taken from ECHA (2021) dossier for Perfluorobutylethylene. Available at: https://echa.europa.eu/registration-dossier/-/registered-dossier/5646/4/23.

In contact with water under dilute conditions, [PFBEMDCS very rapidly (half-life <1 minute at pH 4, pH 7, pH 9 and 20- 25°C) to produce [2-(perfluorobutyl)ethyl](methyl) silanediol and hydrochloric acid according to the following equation (ECHA 2021):

$C_7H_7Cl_2F_9Si + 2H_2O \rightarrow C_7H_9F_9O_2Si + 2HCl$

Literature Search
The following references or databases were searched to identify data to determine the screening level: U.S. Environmental Protection Agency (EPA) Integrated Risk Information System (IRIS), Registry for Toxic Effects of Chemical Substances (RTECS), American Conference of Governmental and Industrial Hygienists (ACGIH) Threshold limit Values (TLVs). International Agency for Research on Cancer (IARC) Monographs, Chemical Abstract Service (CAS) SciFinder (searched 10/28/2020), U.S. EPA ChemView, California Office of Environmental Health Hazard Assessment (OEHHA), and the U.S. Department of Health and Human Services Agency for Toxic Substances and Disease Registry (ATSDR).

Toxicokinetics
Information regarding the absorption, distribution, metabolism, and excretion was not found in the publicly available literature.

Genotoxicity
The only study was found investigating the genotoxicity of PFBEMDCS. This study was conducted using the bacterial reverse mutation assay. Salmonella Typhimurium (strains TA98, TA100, TA1535, TA1537, and E. Coli WP2) were cultured in media containing 78.12, 156.25, 312.5, 625, and 1,250 µg/plate of PFBEMDCS with or without a metabolic activation system. Under the conditions of the test, PFBEMDCS was not found to be mutagenic.

Studies
Acute:
Two acute oral toxicity studies were reported by ECHA (2021). In an OECD 401 compliant study, Sprague-Dawley rats (one male and female/dose) were administered 0.316, 0.63, 1.26, and 2.52 g/kg bw of PFBEMDCS via oral gavage. The initial body weight of the animals ranged from 273 to 307 grams. Clinical signs included lethargy, ataxia, righting response, piloerection, and prostration. No other overt signs of toxicity were noted. All animals administered 1,260 and 2,520 gm/kg bw died. The authors concluded that the LD_{50} was 890 mg/kg bw.

In a supporting guideline compliant study (ECHA 2021), Wistar rats (5/sex/dose) were administered 0; 2,500; 3,000; 3,600; 4,320; and 5,190 mg/kg of PFBEMDCS via oral gavage in a corn oil vehicle. Within a few minutes of the treatment animals showed sluggishness and signs of ataxia. Loss of consciousness occurred in one hour in some rats of the 2,500 and 3,000 mg/kg group and all the 3,600 mg/kg group. Deaths occurred 30 minutes to 2 days after dosing. Survivors appeared healthy at the end of the 14-day recovery period. The LD_{50} was determined to be 2,593 mg/kg.

A skin irritation study reported by ECHA (2021), indicated that PFBEMDCS was corrosive to the abraded and unabraded skin of White New Zealand rabbits. However, the Klimisch rating for this study was four.

Repeat Dose Studies:
No subacute, subchronic, chronic, reproductive, or developmental studies were found in the publicly available literature.

ITSL Derivation
According to Rule 232 (1)(h), the ITSL may be determined from an animal oral LD_{50} as follows:

$$ITSL = 1/500 \times 1/40 \times 1/100 \times \frac{LD50\ mg/kg \times W_A}{0.167 \times I_A}$$

LD_{50} = 890 mg/kg
W_A = Body weight of the experimental animal in kilograms = 0.273-0.307 kg Initial wt.
I_A = Daily inhalation rate of experimental animal in m^3/day using Cal EPA regression model equation[2]
$I = 0.702 \times bw^{2/3}$ in m^3/day or $0.702 \times 0.273^{2/3} = 0.298$ m^3/day and $0.702 \times 0.307^{2/3} = 0.322$ m^3/day of 0.31 m^3/day average

Therefore: $ITSL = 1/500 \times 1/40 \times 1/100 \times \frac{890\ mg/kg \times 0.29\ kg}{0.167 \times 0.31\ m^3/day} = 0.00249\ mg/m^3$

or 2 ug/m^3 (rounded to 1 significant figure). The ITSL is given annual averaging time pursuant to Rule 232(2)(c).

References
ECHA (European Chemical Authority). 2021. Dossier on Perfluorobutylethylmethyldichlorosilane. Available at: https://echa.europa.eu/registration-dossier/-/registered-dossier/21967

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[2] https://oehha.ca.gov/media/downloads/crnr/calcuratbreathingrate092818.pdf