REACH

# 1,1,1,2,2,3,4,5,5,5-decafluoro-3-methoxy-4-(trifluoromethyl)pentane

EC number: 459-520-5 | CAS number: 132182-92-4

Classification & Labelling & PBT assessment

## PBT assessment

S-01 | PBT assessment Summary

## Administrative data

### PBT assessment: overall result

| Reference | |
|---|---|
| Name: | Pentane, 1,1,1,2,2,3,4,5,5,5-decafluoro-3-methoxy-4-(trifluoromethyl)- |
| Type of composition: | legal entity composition of the substance |
| State / form: | liquid |
| Reference substance: | Pentane, 1,1,1,2,2,3,4,5,5,5-decafluoro-3-methoxy-4-(trifluoromethyl)- |

| | |
|---|---|
| PBT status: | the substance is not PBT / vPvB |
| Justification: | The substance is Persistent and very Persistent, but not Bioaccumulative and not Toxic. |



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Environmental fate & pathways

## Endpoint summary

### Administrative data

### Description of key information

### Additional information

HFE s-601 is a segregated hydrofluoroether. It is a liquid at room temperature with a vapor pressure of 6.25 kPa (46.9 mm Hg) at 20 °C and a water solubility of 295 µg/L at 30 °C. Its measured Henry's law constant is 67 atm·m³/mol at 22 °C. The vapor pressure, low water solubility and high Henry's law constant combine to move HFE s-601 from any surface compartment into the atmosphere. Once in the atmospheric compartment, this compound will not partition to terrestrial or aquatic compartments based on the same properties. HFE s-601 was not degraded in either of two OECD301D tests, but was not inhibitory to biodegradation. No biodegradation of HFE s-601 is expected under environmental conditions. Degradation in the environment is expected to occur by indirect photolysis in the troposphere, for which an overall lifetime of 3.8 years was measured. The expected final degradation products are hydrofluoric acid (HF, CAS# 7664-39-3), trifluoroacetic acid (TFA, CAS# 76-05-1) and carbon dioxide. These materials are highly soluble in water and are completely ionized in rainwater. They are expected to undergo wet deposition with no further significant transformation upon return to the troposphere.

HFE s-601 has a measured log Kow of 4.3. Two bioconcentration studies were done, however owing to non-standard and non-representative test conditions these were deemed unreliable and are not considered further. However, HFE s-601 is expected to have little potential to bioaccumulate. Given its extremely short expected half-life in the aquatic compartment due to volatilization, it will not exist in aquatic environments or organisms for a sufficient time to allow partitioning into lipid tissues or testing of bioconcentration under relevant conditions.

As HFE s-601 is a highly fluorinated substance, global warming and ozone depletion potentials may be of interest. USEPA states that hydrofluorocarbons do not deplete ozone because they lack chlorine or bromine. Fluorine radicals do not contribute to ozone depletion because of fast quenching of F* by water or hydrogen donors, slow reaction of FO* radicals with oxygen, and obligate reformation of F* in the pathway (1). F* radicals are rapidly and irreversibly removed from the atmosphere after quenching as HF. Therefore, neither HFE s-601 nor any of its acidic photodegradation products contribute to ozone depletion. Global warming potential depends on three factors: absorption of infrared radiation, area of the spectrum the absorption occurs and lifetime of the material in the atmosphere. HFE s-601 has an estimated GWP of 310 over a 100-year integrated time horizon (2).

Reference:

1) A.J. Colussi, M.A. Crela. 1994. Rate of the reaction between oxygen monofluoride and ozone. Implications for the atmospheric role of fluorine. Chem. Phys. Lett. Vol. 229, pp. 134-138.

2) Registrant internal report.



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### Additional information

HFE s-601 is stable to abiotic degradation. Hydrolysis of HFE s-601 is not expected based on lack of hydrolyzable structural elements. A hydrolysis test was deemed unreliable due to formation of a gas phase in all test vessels by end of test. Indirect phototransformation in the gas phase has a estimated lifetime of 3.8 years based on measured rate constant. The degradation pathway and products of HFE s-601 were not determined. However, the pathway for HFE s-601 in the environment or in vivo can be predicted based on published data for CAS# 297730-93-9 [Hexane, 1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-3-ethoxy-]. CAS# 297730-93-9 differs from HFE s-601 by having one additional difluoromethylene group in the perfluoroalkyl moiety (i.e., a branched perfluoroheptyl group rather than a branched perfluorohexyl group) and by being an ethyl, rather than methyl, ether. Atmospheric fate of CAS# 297730-93-3 was reported in Goto et al., 2002. Using infrared spectroscopy and reactivity characteristics, Goto et al. 2002 proposed a degradative pathway, based on reaction with either hydroxyl or chlorine radical. The first step is oxidation of the non-fluorinated ethyl ether group to either an acetate ester (major product) or formate ester (minor product). This transformation was oxygen dependent. It should be noted that HFE s-601 contains a methoxy, rather than ethoxy, group, and the overall degradation pathway is much simpler. Reactions leading to an acetate ester are not possible, and the formate ester is sole expected product. This is exactly the result found by Wallington, et al. (1997) and Chen et al (2011) for 1 -methoxy 1,1,2,2,3,3,4,4,4-nonafluorobutane (EC# 422-270-2). That is, 1-methoxy 1,1,2,2,3,3,4,4,4-nonafluorobutane was converted to 1,1,2,2,3,3,4,4,4-nonafluorobutyl formate. By analogy, CAS# is 132182-92-4 would be converted to 1,1,1,2,2,3,4,5,5,5-decafluoro-4-(trifluoromethyl)pentyl 3-formate.

The analogous perfluoroalkyl esters were found to be subject to photolysis. Indirect phototransformation of formate esters was found to occur at approximately the same rate as the parents or slower (Wallington et al., 1997; Chen et al., 2011; Goto et al., 2002). In the case of perfluorobutyl formate, the ultimate degradation products were either carbonyl difluoride (from the normal isomer) or a 2:1 mixture of carbonyl difluoride and perfluoroacetyl fluoride (from the isobutyl isomer). Goto et al. did not characterize photodegradation products of the esters. In addition, Chen et al.(2004) examined photolysis of authentic samples of perfluoroethyl and perfluoropropyl formate with hydroxyl radical, whereas perfluorobutyl formate phototransformation was studied on the reaction products of 1-methoxy 1,1,2,2,3,3,4,4,4-nonafluorobutane (Chen et al., 2011). While all cases direct UV photolysis of the esters was significant enough to interfere with their measurements, details sufficient to allow extrapolation from their experimental equipment to direct photolysis in the atmosphere were not provided. In contrast, Nohara et al. (2001) examined photoreaction of a series of methyl perfluoroalkyl ethers with chlorine radicals. The resulting formates were produced in 1:1 molar yield and reacted more slowly than the parent ether molecules. In addition to carbonyl difluoride, a series of perfluoroalkyl fluoride with chain length 1, 2, or 3 carbons shorter than the parent were found through conversion of a perfluoroalkoxy radical to a perfluorinated alcohol and subsequent dehydrofluorination (it should be noted that this process depends on presence of HO2 and would occur in air with high levels of photooxidants). Such a reaction sequence is not possible for HFE s-601 as only one fluorine atom is in the geminal position. Dehydrofluorination can proceed only as far as a ketone, not a carboxylic acid (see below)

The hydrolytic instability of perfluoroalkyl esters due to inductive effects of the fluorine substituent has long been known (Pavlik and Toren, 1970). Uchimara et al. (2003) performed ab initio calculations on fluorinated and non-fluorinated methyl acetate compounds. They concluded that inductive effects of fluorine substitution would stabilize the tetrahedral hydrolysis intermediate and increase the reaction rate. They speculated that neutral hydrolysis may also be potentiated by induction. Therefore, hydrolysis of dissolved ester is likely to occur on a timescale of minutes. Hydrolysis of the ester from HFE s-601 would lead to a perfluorinated secondary alcohol. Perfluorinated alcohols undergo spontaneous dehydrofluorination as noted earlier. In the case of a secondary alcohol, this process can proceed only to the formation of a ketone. For HFE s-601 phototransformation products dehydrofluorination leads to 1,1,1,2,2,4,5,5,5-nonafluoro-4-(trifluoromethyl)-3-pentanone (CAS# 756-13-8). This material is registered under REACH and its photolytic and hydrolytic products are well known.

In two closed-bottle tests of biodegradability, no biodegradation of HFE s-601 was observed. This suggests that metabolism of HFE s-601 in vivo is not likely. In the unlikely event that biologically mediated oxidation were to occur, oxidase activity would be centered on the methoxy group similar to what has been observed in phototransformation experiments.

Chen L, Kutsuna S, Tokuhashi K, Sekiya A. 2004. Kinetics study of the gas-phase reactions of C2F5OC(O)H and n-C3F7OC(O)H with OH radicals at 253–328 K. Chem. Phys. Lett. (400) 563-568.

Chen L, Uchimaru T, Kutsuna S, Tokuhashi K, Sekiya A. 2011. Kinetics and mechanism of gas-phase reactions of n-C4F9OCH3, i-C4F9OCH3, n-C4F9OC(O)H, and i-C4F9OC(O)H with OH radicals in an environmental reaction chamber at 253–328 K. Chemical Physics Letters (514) 207-213

Goto M, Inoue Y, Kawasaki M, Guschin AG, Molina LT, Molina MJ, Wallington TJ, Hurley MD. 2002. Atmospheric Chemistry of HFE-7500 [n-C3F7CF(OC2H5)CF(CF3)2]: Reaction with OH Radicals and Cl Atoms and Atmospheric Fate of n-C3F7CF(OCHO·)CF(CF3)2 and n-C3F7CF(OCH2CH2O·)CF(CF3)2 Radicals. Environ. Sci. Technol. (36) 2395-2402

Nohara K. Toma M, Kutsuna S, Takeuchi K, Ibusuki T. 2001. Cl atom-initiated oxidation of three homologous methyl perfluoroalkyl ethers. Environ. Sci. Technol. (35) 114-120.

Pavlik J, Toren PE. 1970. Perfluoro-t-butyl Alcohol and its Esters. J. Org. Chem. (35) 2054-2056.

Uchimaru T, Kutsuna S, Chandra AK, Sugie M, Sekiya A. 2003. Effect of fluorine substitution on the rate for ester hydrolysis: estimation of the hydrolysis rate of perfluoroalkyl esters. J. Mol. Structure (Theochem) (635) 83-89.

Wallington TJ, Schneider WF, Sehestad J, Bilde M, Platz J, Nielsen OJ, Christensen LK, Molina MJ, Molina LT, Wooldridge PW. 1997. Atmospheric Chemistry of HFE-7100 (C4F9OCH3): Reaction with OH Radicals, UV Spectra and Kinetic Data for C4F9OCH2· and C4F9OCH2O2· Radicals, and the Atmospheric Fate of C4F9OCH2O· Radicals. J. Phys. Chem. A (101) 8264-8274

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Environmental fate & pathways

## Endpoint summary

### Administrative data

### Description of key information

### Additional information

HFE s-601 is stable to biodegradation. No oxygen depletion was measured in two closed bottle tests (OECD 301D), and measured concentrations of test substance did not change in the test for which analytical determination of test substance concentration was included in the test procedure. Biodegradation in the environment is expected to be very slow to non-existent.



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Environmental fate & pathways

## Bioaccumulation: aquatic / sediment

S-01 | Summary

### Administrative data

### Link to relevant study record(s)

### Description of key information

### Key value for chemical safety assessment

### Additional information

Bioaccumulation of HFE 601 was examined in two studies, a preliminary test conducted with limited scope and a final test with a larger sample size and more time points. Both studies were based on OECD 305 methods and used flow-through exposure. However, both studies used a cosolvent and a dispersing aid. Neither agent is approved for use in OECD 305. In particular, the dispersing aid was a perfluorooctanesulfonamide-based surfactant, which is not appropriate or relevant for biological systems. The combination of both agents is irregular, and neither study is considered reliable. Both studies are disregarded. However, a measured Henry's Law constant of 2770 at 22 °C (dimensionless. In standard units, 6.79E+06 Pa·m³/mol) indicates that HFE 602 is not compatible with aqueous solution and will rapidly volatilize from any open system. Bioaccumulation of HFE 602 is not expected in natural aquatic systems due to lack of exposure caused by extreme volatility.

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Ecotoxicological information

## Ecotoxicological Summary

### Administrative data

### Hazard for aquatic organisms

#### Freshwater

Hazard assessment conclusion: no hazard identified

#### Marine water

Hazard assessment conclusion: no hazard identified

#### STP

Hazard assessment conclusion: no hazard identified

#### Sediment (freshwater)

Hazard assessment conclusion: no hazard identified

#### Sediment (marine water)

Hazard assessment conclusion: no hazard identified

### Hazard for air

#### Air

Hazard assessment conclusion: no hazard identified

### Hazard for terrestrial organisms

#### Soil

Hazard assessment conclusion: no hazard identified

### Hazard for predators

#### Secondary poisoning

no potential for bioaccumulation

Hazard assessment conclusion:

Additional information

## Conclusion on classification

Environmental classification justification:

CLP acute: Conclusive although insufficient for classification

CLP chronic: Conclusive althugh insufficient for classification

No toxicity at limit of water solubility for fish, Daphnia or algae; high volatility; no long-term presence in the aquatic compartment

HFE s-601 is not listed in the Montreal Protocol on Substances that Deplete the Ozone Layer. It does not contain reactive halogens (chlorine or bromine) that could play a role in ozone depletion. HFE s-601 is not hazardous to the ozone layer

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Toxicological information

## Toxicological Summary

### Administrative data

### Workers - Hazard via inhalation route

#### Systemic effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

**DNEL related information**

#### Local effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

**DNEL related information**

### Workers - Hazard via dermal route

#### Systemic effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

**DNEL related information**

#### Local effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

## Workers - Hazard for the eyes

### Local effects

Hazard assessment conclusion: no hazard identified

## Additional information - workers

## General Population - Hazard via inhalation route

### Systemic effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

**DNEL related information**

### Local effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

**DNEL related information**

## General Population - Hazard via dermal route

### Systemic effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

**DNEL related information**

### Local effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

## General Population - Hazard via oral route

### Systemic effects

**Long term exposure**

Hazard assessment conclusion: no hazard identified

**Acute/short term exposure**

Hazard assessment conclusion: no hazard identified

**DNEL related information**

## General Population - Hazard for the eyes

### Local effects

| | |
|---|---|
| Hazard assessment conclusion: | no hazard identified |

## Additional information - General Population