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REACH

2-Pentene, 1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)-, (E)-

EC number: 807-113-1 ; CAS number: 3709-71-5

Substance identity

Identification

Display Name:	2-Pentene, 1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)-, (E)-
EC Number:	807-113-1
CAS Number:	3709-71-5
Molecular formula:	C6F12
IUPAC Name:	2-Pentene, 1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)-, (E)-

Type of Substance

Composition:	mono-constituent substance
Origin:	organic

Substance Identifiers

Compositions

Boundary Composition(s)

HFP-Dimer

State Form: liquid

Constituent 1

Reference substance name:	2-Pentene, 1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)-, (E)-
EC Number:	807-113-1
CAS Number:	3709-71-5
Molecular formula:	C6F12
IUPAC Name:	2-Pentene, 1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)-, (E)-

Legal Entity Composition(s)

HFP-Dimer

State Form: liquid

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EC number: 807-113-1 ⋮ CAS number: 3709-71-5

Classification & Labelling & PBT assessment

PBT assessment

S-01 | PBT assessment Summary

Administrative data

PBT assessment: overall result

PBT status:	the substance is not PBT / vPvB
Justification:	All impurities identified as present in HFP kinetic dimer at > or = 0.1% are isomers or homologues of HFP kinetic dimer, with physical/chemical properties essentially the same as HFP kinetic dimer. Impurities therefore have PBT characteristics equivalent to HFP kinetic dimer. The ultimate degradation products are expected to be hydrofluoric acid, trifluoroacetic acid, isoperfluorobutyric acid and carbon dioxide. HF and CO2 are inorganic substances not needing a PBT assessment and TFA and PFBA are not bioconcentrating or toxic. By screening and definitive REACH PBT criteria, HFP kinetic dimer is very persistent, "vP". An evaluation of its fate in water or soil concludes that HFP kinetic dimer is rapidly removed to the atmospheric compartment by volatilization, and it will not partition into water or soil from the atmosphere. Therefore, this substance is non-persistent in the aquatic and terrestrial environments. It is very persistent only in the atmosphere and is subject to long-range transport in the atmosphere but is not subject to deposition in remote or pristine environments. Due to mixing in the atmosphere and lack of partitioning out of the atmosphere, concentrations in the biosphere will be negligible. Widespread exposure to HFP kinetic dimer will not occur. Based on the expected partitioning behavior of HFP kinetic dimer, additional laboratory studies on the biodegradation and bioaccumulation in the water, sediment and soil compartments are not relevant for the evaluation of PBT properties of this substance. The "B" criterion in aquatic organisms is not met due to lack of exposure. The calculated log Koa value indicates that HFP kinetic dimer cannot bioaccumulate in air-breathing animals. Collectively, the log Kow, the HLC, and the calculated Koa indicate that HFP kinetic dimer is not expected to bioaccumulate in aquatic, sediment or soil organisms. HFP kinetic dimer does not fulfill the criteria for bioaccumulative ("B") or very bioaccumulative ("vB"). Based on available data, HFP kinetic dimer is not classified as carcinogenic, mutagenic, or toxic to reproduction or specific target organ toxic after repeated dose. HFP kinetic dimer does not meet the REACH "T" criteria for mammalian toxicity. This information combined with the lack of acute aquatic toxicity can be used to conclude that HFP kinetic dimer does not fulfill the screening criteria for toxic ("T"). The data show that the properties of the substance do NOT meet the specific criteria in Annex XIII Section 1, or while not allowing a direct comparison with all the

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REACH

2-Pentene, 1,1,1,2,3,4,5,5,5-nonafluoro-4-(trifluoromethyl)-, (E)-

EC number: 807-113-1 | CAS number: 3709-71-5

Ecotoxicological information

Ecotoxicological Summary

Administrative data

Hazard for aquatic organisms

Freshwater

Hazard assessment conclusion:	PNEC aqua (freshwater)
PNEC value:	0.012 µg/L
Assessment factor:	1 000

Marine water

Hazard assessment conclusion:	PNEC aqua (marine water)
PNEC value:	0.001 µg/L
Assessment factor:	10 000

STP

Hazard assessment conclusion:	PNEC STP
PNEC value:	10 mg/L
Assessment factor:	100

Sediment (freshwater)

Hazard assessment conclusion:	PNEC sediment (freshwater)
PNEC value:	3.16 µg/kg sediment dw
Extrapolation method:	equilibrium partitioning method

Sediment (marine water)

Hazard assessment conclusion:	PNEC sediment (marine water)
PNEC value:	0.316 µg/kg sediment dw
Extrapolation method:	equilibrium partitioning method

Hazard for air

Air

PNEC air

most sensitive long-term study result (0.83 mg/kg dry weight in soil), to derive a PNECsoil of 0.0083 mg/kg. TFA is expected to remain in the soil water and not sorb to soil. Plants exposed hydroponically showed more sensitivity than those where soil was dosed. PNEC was also determined using the equilibrium partitioning method (EPM) and the freshwater PNEC: PNECsoil = (0.174 + (0.0104 x Koc)) x PNECwater, where the Koc was 0.023 and the freshwater PNEC was 0.0064 mg/L. This value was then converted to dry weight: (PNEC mg/kg ww) x 1.13 = PNEC of 0.0013 mg/kg dry weight. The PNEC derived using the equilibrium method was lower than that derived using application factors. Because this value was the lesser of the two and because TFA is expected to remain in the soil water, the PNEC derived with the EPM method, 0.0013 mg/kg dw, will be the definitive value. TFA is not readily biodegradable. However, Bioconcentration was evaluated using TFA uptake data from several aquatic studies and terrestrial plant studies (1). BCF values ranged from 1.0 - 43. It is thought that uptake into terrestrial plants is in part due to translocation of dissolved TFA in the tissue water (1). None of these studies demonstrated that TFA would be considered bioaccumulative. In addition, the log Kow was reported to be -2.1. Therefore, bioaccumulation of TFA in terrestrial or aquatic organisms is not expected and secondary poisoning does not need to be considered further in this assessment.

(1)Boutonnet (Ed.), 1999. Environmental Risk Assessment of Trifluoroacetic Acid. Human and Ecological Risk Assessment: Vol. 5, No. 1, pp. 59-124.

(2) Mark L. Hanson, Keith R. Solomon. Haloacetic acids in the aquatic environment.Part I: macrophyte toxicity. Environmental Pollution 130 (2004) 371-383

(3) Benesch, J.A. et al., 2002. Investigation of effects of trifluoroacetate on vernal pool ecosystems. Environmental Toxicology and Chemistry, Vol. 21, No. 3, pp. 640-647.

Iso Perfluorobutyric acid (CAS 335-10-4): Using available aquatic toxicity data, the freshwater PNEC was found to be 2.6 mg/L and the marine PNEC 0.26 mg/L. Acute results from testing perfluorobutyric acid were available for 12 species in at least three taxonomic groups and chronic for three species in two taxonomic groups. As per R.10, Table R.10-4 footnote (d): one can reduce the AF to 10 in cases where it is possible to determine with high probability that the most sensitive species has been examined, i.e. that a further long-term result (e.g. EC10 or NOEC) from a different taxonomic group would not be lower than the data already available. This is also appropriate because perfluorobutyric acid does not bioaccumulate (BCF reported as < 3 - 6 at the 0.02 mg/L exposure and < 28 at the 0.2 mg/L exposure in a BCF test with carp). P. subcapitata has an ErC50 nearly one order of magnitude lower than and a NOEC more than one order of magnitude lower than all other organisms tested, including the green alga C. vulgaris. This extreme sensitivity of P. subcapitata has been seen with other small chain pefluorinated acids (i.e. trifluoroacetic acid). An AF of 10 will be taken in this case due to the evidence from the large data set for this substance and the evidence for testing with trifluoroacetic acid. For the calculation of the Freshwater PNEC a 72-hour ErC10 value of 26 mg/L was obtained from a study with Pseudokirchneriella subcapitata. An AF of 10 was applied to this algae ErC10. There is no additional data available on marine taxonomic groups. An additional factor of 10 was applied to the Freshwater PNEC to derive the Marine Water PNEC. For the STP PNEC, a NOEC of 1000 mg/L was available for activated sludge respiration inhibition. An assessment factor of 10 was applied to the NOEC to derive a PNEC of 100 mg/L for STP. No test results for freshwater sediment were available. PNEC was extrapolated using the equilibrium partitioning method (EPM) with the freshwater PNEC. PNECsed = (0.783 + (0.0217 x Koc)) x PNECfreshwater, where the Koc was 1.0 L/kg and the freshwater PNEC was 2.6 mg/L. PNEC converted to dry weight: (PNEC mg/kg ww) x 4.6 = PNEC of 9.61 mg/kg dry wt. No test results for Marine Sediment were available. PNEC was extrapolated using the equilibrium partitioning method (EPM) with the marine PNEC. PNECmarinesed = (0.783 + (0.0217 x Koc)) x PNECmarinewater, where the Koc was 1.0 L/kg and the marine PNEC was 0.26 mg/L. PNEC converted to dry weight: (PNEC mg/kg ww) x 4.6 = PNEC of 0.961 mg/kg dry wt.

No experimental data available on air. As this study is not a standard information requirement in REACH and there is no indication from the CSA on the need to investigate further the atmospheric compartment, no PNEC was derived. No test results for Soil were available. PNEC was extrapolated using the equilibrium partitioning method (EPM) including the freshwater PNEC, PNECsoil = (0.174 + (0.0104 x Koc)) x PNECwater, where the Koc was 1.0 L/kg and the freshwater PNEC was 2.6 mg/L. PNEC converted to dry weight: (PNEC mg/kg ww) x 1.13 = PNEC of 0.541 mg/kg dry weight. Although PFBA is not readily biodegradable, the bioconcentration factor was found to be < 28 in a laboratory study with fish. This substance is not considered bioaccumulative. Therefore, the PNEC oral is not applicable and was not derived.

Conclusion on classification

For HFP Kinetic Dimer:

CLP Aquatic acute: Acute 1

M-Factor: 10

Aquatic chronic: Chronic 2

M-factor chronic: N/A

Ozone Depletion: HFP Kinetic Dimer 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. HFP Kinetic Dimer is not hazardous to the ozone layer. Conclusive although not sufficient for classification.

Trifluoroacetic acid degradation product (CAS# 76 -05 -01):

CLP: Aquatic acute: Not classified - conclusive although not sufficient for classification.

M-factor acute: N/A

Aquatic Chronic 3

M-factor chronic: N/A

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EC number: 807-113-1 | CAS number: 3709-71-5

Environmental fate & pathways

Endpoint summary

Administrative data

Description of key information

Additional information

HFP kinetic dimer is used as a process aid for polymer manufacture. HFP kinetic dimer is a liquid at room temperature with a vapor pressure of 34.7 kPa at 20°C. The water solubility is 649 µg/L at 22.3 °C. The measured Henry's Law constant (HLC) is 1.40E+07 Pa·m³/mol (138 atm·m³/mole). The vapor pressure, low water solubility and high Henry's law constant combine to move HFP kinetic dimer from any terrestrial compartment into the atmosphere. Evaporation of HFP kinetic dimer from surfaces is rapid. Fugacity modeling indicates that distribution from soil to air dominates over all other processes, and therefore that release to soils would result in rapid volatilization to the atmospheric compartment. Because articles containing the substance are only used indoors, the substance is not exposed to weathering; essentially all releases are to the atmospheric compartment. Assuming 100% release to the atmospheric compartment, 99.996% of substance remains in the gas phase of the air compartment, with 0.0036% in gas-filled pore paces, and 0.00020% sorbed to soil solids. Therefore, this compound will remain in the atmosphere when released from industrial applications. However, disposal of articles at the end of their service life may be by landfill. In the worst case, with 100% of HFP kinetic dimer emission directed to the soil compartment, 97.9% of HFP kinetic dimer was predicted to be in the gas phase in the air compartment, whereas 2.0% was predicted to be in the gas-filled pore spaces in the soil, and 0.11% sorbed to soil solid. It is not biodegradable, and hydrolysis is not expected to contribute to environmental degradation. Degradation in the environment is by indirect photolysis, with a half-life of approximately 0.57 years (overall atmospheric lifetime, 0.82 years). The pathway for decay is expected to be analogous to that for perfluorobutene (1), i.e., addition of hydroxyl radical to the unsaturated group followed by scission to form a carboxylate moiety from each of the two unsaturated carbons. The ultimate degradation products are expected to be perfluoroisobutyric acid (i-PFBA, CAS# 335-10-4), trifluoroacetic acid (TFA, CAS# 76-05-1) and hydrofluoric acid (HF, CAS# 7664-39-3). These acids are miscible in water and are completely ionized in rainwater. They are expected to undergo wet deposition with no further significant transformation. Please note that a published environmental risk assessment on TFA is available in the literature (2).

USEPA states flatly that fluorocarbons 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 (3). F* radicals are rapidly and irreversibly removed from the atmosphere after quenching as HF. Therefore, neither HFP kinetic dimer nor any of its acidic photodegradation products contribute to ozone depletion.

HFP kinetic dimer is not expected to partition to moist soils or surface waters. Upon accidental, direct release to the aquatic compartment, the chemical is expected to volatilize rapidly. In closed-bottle (OECD301D) assays, ≤12% biodegradation was observed. HFP kinetic dimer has a measured n-octanol: water partition coefficient of 4.1 and is expected to have little potential to bioaccumulate. The calculated log Koa of HFP kinetic dimer is 0.39. This log Koa value indicates that HFP kinetic dimer has a low potential to partition from air to the lipid rich tissues of air-breathing organisms. Given its extremely short half-life due to volatilization, it would not remain in aquatic environments or organisms for a sufficient time to allow partitioning into lipid tissues or to permit meaningful testing of bioconcentration.

Partitioning of i-PFBA, TFA, and HF in the environment is driven by the fact that these acids are completely ionized at environmental pH values, are miscible in water, and are not likely to bind with organic matter based on low Koc values and low log Kow values. i-PFBA, TFA, and HF will be associated with the aqueous phase of any environment where they are released, and will be highly mobile in soils. i-PFBA, TFA, and HF that have deposited in aquatic compartments are expected to remain in the aquatic compartment.

The registrant is not aware of information on biodegradation of i-PFBA. The registrant has assessed perfluoropropanoic acid (PFPA) in ready biodegradation tests and demonstrated that essentially no biodegradation occurs. TFA (see below) is similarly not biodegraded. Based on results from other internally-conducted studies of longer chain perfluorinated chemicals, it is anticipated that

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EC number: 807-113-1 ; CAS number: 3709-71-5

Toxicological information

Toxicological Summary

Administrative data

Workers - Hazard via inhalation route

Systemic effects

Long term exposure

Hazard assessment conclusion:	DNEL (Derived No Effect Level)
Value:	270 mg/m³
Most sensitive endpoint:	repeated dose toxicity
Route of original study:	By inhalation

DNEL related information

DNEL derivation method:	ECHA REACH Guidance
Overall assessment factor (AF):	12.5
Dose descriptor starting point:	NOAEC
Value:	6 748.5 mg/m³
Modified dose descriptor starting point:	NOAEC
Value:	3 386.5 mg/m³
Explanation for the modification of the dose descriptor starting point:	The dose descriptor was multiplied by 6/8 to account for 6 hour dosing per day compared to an 8 hour workday, and then by .67 for work activity.
AF for interspecies differences (allometric scaling):	2.5
AF for intraspecies differences:	5

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

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: hazard unknown but no further hazard information necessary as no exposure expected

Acute/short term exposure

Hazard assessment conclusion: hazard unknown but no further hazard information necessary as no exposure expected

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: hazard unknown but no further hazard information necessary as no exposure expected

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

Information on Registered Substances comes from registration dossiers which have been assigned a registration number. The assignment of a registration number does however not guarantee that the information in the dossier is correct or that the dossier is compliant with Regulation (EC) No 1907/2006 (the REACH Regulation). This information has not been reviewed or verified by the Agency or any other authority. The content is subject to change without prior notice.

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