Justification Document for the Selection of a CoRAP Substance

Substance Name (public name):	3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)hexane
EC Number:	435-790-1 /608-415-4
CAS Number:	297730-93-9
Authority:	Spain (CA-ENV)
Date:	20/03/2018

Cover Note

This document has been prepared by the evaluating Member State given in the CoRAP update.

Table of Contents

1 IDENTITY OF THE SUBSTANCE

Please refer to public information from ECHA dissemination website whenever available.

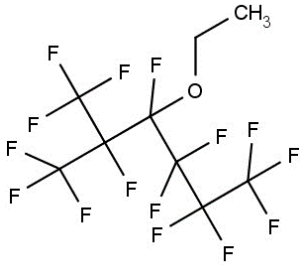
1.1 Other identifiers of the substance

Table: Other Substance identifiers

EC name (public):	3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane
IUPAC name (public):	3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane
Index number in Annex VI of the CLP Regulation:	603-224-00-2
Molecular formula:	C9H5F15O
Molecular weight or molecular weight range:	414.114 g/mol
Synonyms:	HFE-7500 ENGINEERED FLUID
smiles	CCOC(C(C(F)(F)F)(C(F)(F)F)F)(C(C(C(F)(F)F)(F)F)(F)F)F

Type of substance ☒ Mono-constituent ☐ Multi-constituent ☐ UVCB

Structural formula:



Physical state: clear, colourless liquid at 20°C and 1013 hPa

Other relevant information about substance composition

There is no other relevant information about substance composition

1.2 Similar substances/grouping possibilities

Has read-across been used by the registrant for the concern related endpoints? ☒ Yes ☐ No

Is the substance a member of a category? ☒ Yes ☐ No

The substance is a member of the hydrofluoroethers (HFEs) group.

297730-93-9 HFE 7500

PBT Profiler Estimate = PBT

Screening estimates indicate this chemical may be a PBT - a P2 Assessment may allow further evaluation

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	180	5%	4,700	0.021
Soil	360	0%		
Sediment	1,600	90%		
Air	24	4%		

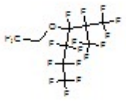


Table: Identified Hydrofluoroethers (HFEs)

IUPAC name	HFEs	CAS number	EC number	Mol formula	MW	Principal probable uses
	HFE-125	3822-68-2	-	CF3OCF2H	136	Refrigerant
	HFE-134	1691-17-4	-	CHF2OCHF2	118	Refrigerant, blowing agent
	HFE-143a	421-14-7	-	CF3OCH3	100	Refrigerant
	HFE-227me	2356-62-9	-	CF3OCFHCF3	186	Dry etching agent, refrigerant
	HFE-245mf	1885-48-9	-	CF3CH2OCF2H	150	Blowing agent, refrigerant
	HFE-245mc	22410-44-2	-	CF3CF2OCH3	150	Refrigerant, blowing agent
1,1,2,2-tetrafluoro-1-methoxyethane	HFE-254pc	425-88-7	207-039-4*	CHF2CF2OCH3	132	Refrigerant, blowing agent
1,1,2,3,3,3-Hexafluoropropyl Methyl Ether	HFE-356mec	382-34-3	609-536-5*	CF3CHFCF2OCH3	182	Blowing agent, refrigerant
Bis(2,2,2-trifluoroethyl) Ether	HFE-356mff	333-36-8	626-793-9**	CF3CH2OCH2CF3	182	Refrigerant

Confidential information	HFE-7000 (NONS subs)		484-450-7	Confidential information	Confidential information	Confidential information
Propane, 1,1,1,2,2,3,3-heptafluoro-3-methoxy-	HFE-7000 (HFE-347mcc)	375-03-1	609-440-3*	n-C3F7OCH3	200	Cleaning solvent, refrigerant
1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane; 1,1,1,2,3,3-hexafluoro-3-methoxy-2-(trifluoromethyl)propane	HFE-7100		422-270-2	C4F9OCH3	250	Cleaning solvent
Hydrofluor ether	HFE-7100 (HFE-449mccc)	163702-08-7	605-340-9*	C4F9OCH3	250	Cleaning solvent
		163702-07-6	605-339-3*			
Butane, 1-ethoxy-1,1,2,2,3,3,4,4,4-nonafluoro-	HFE-7200 (HFE-569mccc)	163702-05-4	605-340-9* 922-358-5 *			
Ethyl nonafluoroisobutyl ether		163702-06-5	639-027-3**	C4F9OC2H5	264	Cleaning solvent
Confidential information	HFE-7800		Confidential information	Confidential information	Confidential information	Confidential information

- not included at the ECHA dissemination site; *Pre-registered under REACH Regulation; ** Not pre-registered nor registered.

2 OVERVIEW OF OTHER PROCESSES / EU LEGISLATION

Table: Completed or ongoing processes

RMOA		☐ Risk Management Option Analysis (RMOA)
REACH Processes	Evaluation	☐ Compliance check, Final decision
		☐ Testing proposal, Final decison
		☐ CoRAP and Substance Evaluation
	Authorisation	☐ Candidate List
		☐ Annex XIV
	Restri	☐ Annex XVII[1]
Harmonised C&L		☒ Annex VI (CLP) (see section 3.1)
Processes under other EU legislation		☐ Plant Protection Products Regulation Regulation (EC) No 1107/2009
		☐ Biocidal Product Regulation Regulation (EU) 528/2012 and amendments
Previous legislation		☐ Dangerous substances Directive Directive 67/548/EEC (NONS)
		☐ Existing Substances Regulation Regulation 793/93/EEC (RAR/RRS)
(UNEP) Stockholm convention (POPs Protocol)		☐ Assessment
		☐ In relevant Annex

[1] Please specify the relevant entry.

Other processes / EU legislation	☐ Other (provide further details below)

3 HAZARD INFORMATION (INCLUDING CLASSIFICATION)

3.1 Classification

3.1.1 Harmonised Classification in Annex VI of the CLP

Table: Harmonised classification

Index No	International Chemical Identification	EC No	CAS No	Classification		Spec. Conc. Limits, M-factors	Notes
				Hazard Class and Category Code(s)	Hazard statement code(s)		
603-224-00-2	3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane	435-790-1	29773 0-93-9	Aquatic Chronic 4	H413		

3.1.2 Self classification

- In the registration: None
- The following hazard classes are in addition notified among the aggregated self classifications in the C&L Inventory: None

3.1.3 Proposal for Harmonised Classification in Annex VI of the CLP

No applicable.

4 INFORMATION ON (AGGREGATED) TONNAGE AND USES[2]

4.1 Tonnage and registration status

Table: Tonnage and registration status

From ECHA dissemination site		
☒ Full registration(s) (Art. 10)	☐ Intermediate registration(s) (Art. 17 and/or 18)	
Tonnage band (as per dissemination site)		
☐ 1 – 10 tpa	☐ 10 – 100 tpa	☐ 100 – 1000 tpa
☐ 1000 – 10,000 tpa	☐ 10,000 – 100,000 tpa	☐ 100,000 – 1,000,000 tpa
☐ 1,000,000 – 10,000,000 tpa	☐ 10,000,000 – 100,000,000 tpa	☐ > 100,000,000 tpa
☒ 10+ tpa		☐ Confidential
Only one registrant with data from 2011.		

4.2 Overview of uses

Hydrofluoroethers (HFEs) are being used as third generation replacements to chlorofluorocarbons (CFCs), hydrochlorofluorocarbons HCFCs) and perfluorocarbons (PFCs) because of their nearly zero stratospheric ozone depletion and relatively low global warming potential.

Their commercial and industrial uses regards as refrigerant, cleaning solvent, foaming agent and dry etching agent (see also table in section 1.2):

- Refrigernts: CFCs were used in domestic refrigerators, freezers and air conditioners. As these substances have been targeted as GHGs in the Kyoto Protocol, HFEs will gradually increase with its more extensive applications because of their lower cost than HFCs.

- Cleaning solvent: it is necessary to use HFCs (phase-out under Montreal Protocol) or HFEs as cleaning solvents in the some precision processes or equipments. HFE 7500 among others HFEs could be termed as dense non-aqueous phase liquid (DNAPL), examples of which could include trichloroethylene and perchloroethylene, from a leakage or illegal dumping.

[2] *The dissemination site was accessed in October 2017.*

- Blowing agent: According to the thermal conductivity, some HFEs are potential alternatives to the traditional blowing agents (CFCs).
- Dry etching agent (process of removing exposed SiO 2 thin-film in the pattern formed by photoresist exposure and development) : used in substitution of PFCs in semiconductor industry.
- Other applications: carrier solvents for coatings, and lubricants or friction-reduction agents on devices such as surgical knife blades

Table: Uses

Part 1:

☒ Manufacture	☐ Formulation	☒ Industrial use	☒ Professional use	☐ Consumer use	☒ Article service life	☐ Closed system

Part 2:

	Use(s)
Uses as intermediate	
Formulation	
Uses at industrial sites	ERC 7: Industrial use of substances in closed systems PROC 1: Use in closed process, no likelihood of exposure, PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities
Uses by professional workers	ERC 9a: Wide dispersive indoor use of substances in closed systems, PROC 8b: Transfer of substance or preparation (charging/discharging) from/to vessels/large containers at dedicated facilities, PROC 1: Use in closed process, no likelihood of exposure
Consumer Uses	
Article service life	

Release to the environment of this substance is likely to occur from industrial use: manufacturing of the substance. The substance is manufactured in closed redestillation systems.

Release to the environment of this substance is likely to occur from industrial use: of substances in closed systems with minimal release.

Other release to the environment of this substance is likely to occur from: indoor use in close systems with minimal release (e.g. cooling liquids in refrigerators, oil-based electric heaters).

Part 3: There is high potential for exposure of

☐ Humans	☒ Environment

5 JUSTIFICATION FOR THE SELECTION OF THE CANDIDATE CORAP SUBSTANCE

5.1 Legal basis for the proposal

☒ Article 44(2) (refined prioritisation criteria for substance evaluation)

☐ Article 45(5) (Member State priority)

5.2. Selection criteria met (why the substance qualifies for being in CoRAP)

☐ Fulfils criteria as CMR/ Suspected CMR

☐ Fulfils criteria as Sensitiser/ Suspected sensitiser

☐ Fulfils criteria as potential endocrine disrupter

☒ Fulfils criteria as PBT/vPvB / Suspected PBT/vPvB

☐ Fulfils criteria high (aggregated) tonnage (*tpa > 1000*)

☒ Fulfils exposure criteria

☐ Fulfils MS's (national) priorities

5.3 Initial grounds for concern to be clarified under Substance Evaluation

Hazard based concerns		
CMR ☐ C ☐ M ☐ R	Suspected CMR[1] ☐ C ☐ M ☐ R	☐ Potential endocrine disruptor
☐ Sensitiser	☐ Suspected Sensitiser[3]	
☐ PBT/vPvB	☒ Suspected PBT/vPvB[1]	☐ Other (please specify below)
Exposure/risk based concerns		
☒ Wide dispersive use	☐ Consumer use	☐ Exposure of sensitive populations
☒ Exposure of environment	☐ Exposure of workers	☐ Cumulative exposure
☐ High RCR	☐ High (aggregated) tonnage	☐ Other (please specify below)

[3] CMR/Sensitiser: known carcinogenic and/or mutagenic and/or reprotoxic properties/known sensitising properties (according to CLP harmonized or registrant self-classification or CLP Inventory)

In an OECD 301D test with 3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane, only 1-2 % degradation was observed after 28 days (based on O_2 consumption). Hence, the substance is not readily biodegradable. In experimental photolysis studies (not following any guidelines), atmospheric half-lives of 1.5-2 years in the presence of hydroxyl or chlorine radicals were estimated for the substance, and n-C3F7CF(OC(O)CH3)CF(CF3)2 and n-C3F7CF(OC(O)H)CF(CF3)2 were identified as degradation products in the presence of chlorine radicals. There is no further experimental information available on the degradation of the substance.

The available data do not allow assessing degradation in environmental compartments. However, the substance has a perfluorinated carbon chain and it is known that PFCs in general are persistent in the environment. Furtermore, based on EPISUITE BIOWIN QSAR models, the substance as well as the degradation products identified in the photolysis study are not readily biodegradable. Therefore, the substance is considered to be potentially persistent or very persistent.

Due to its volatility 3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane may have a potential for long range transport.

The available experimental bioconcentration factors in fish range between 3150 and 8530 L/kg. 3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane is therefore considered to be potentially bioaccumulative or very bioaccumulative.

The substance is classified as Aquatic chronic 4. Only short-term toxicity studies on fish are available for 3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane. In these studies no effects were observed at the limit of the water solubility. However, due to the low water solubility of the substance, long-term studies are needed to assess the aquatic toxicity.

The registration dossier includes also short-term studies on fish, aquatic invertebrates and algae and a long-term study on daphnia performed with perfluorobutyric acid (or its salt) (PFBA) which resulted in low or no toxicity. According to the registrant information (at the ECHA dissemination site) this substance could be a potential degradation product of 3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane (see information on the section "reference substance"). But no mention on degradation products is specifically referred at the section "degradation".

The PBT profiler estimates a NOEC of 0.021 mg/L for fish. Based on the available information, T requires further in depth evaluation.

In conclusion, 3-ethoxy-1,1,1,2,3,4,4,5,5,6,6,6-dodecafluoro-2-(trifluoromethyl)-hexane fulfills the screening criteria for persistence and is potentially bioaccumulative/very bioaccumulative as defined in Annex XIII of REACH.

5.4 Preliminary indication of information that may need to be requested to clarify the concern

☐ Information on toxicological properties	☐ Information on physico-chemical properties
☒ Information on fate and behaviour	☐ Information on exposure
☒ Information on ecotoxicological properties	☐ Information on uses

Suspected CMR/Suspected sensitiser: suspected carcinogenic and/or mutagenic and/or reprotoxic properties/suspected sensitising properties (not classified according to CLP harmonized or registrant self-classification)
Suspected PBT: Potentially Persistent, Bioaccumulative and Toxic

☐ Information on ED potential	☐ Other (provide further details below)

Further evaluation and, if necessary, further testing is required to clarify whether the substance is persistent or very persistent.

Further evaluation and, if necessary, further testing is required to clarify whether the substance is toxic.

5.5 Potential follow-up and link to risk management

☐ Harmonised C&L	☒ Restriction	☒ Authorisation	☐ Other (provide further details)

If the substance is identified as a PBT/vPvB substance, an analysis of risk management options will be carried out, taking into account information on use and exposure. Potential options are the inclusion in the Candidate List with or without Authorisation, but also Restriction.