# Deliverable report for:

# Advice on environmental distribution profile of

# <u>"FC-770"</u>

# (EC number: 473-390-7)

Rapporteur: Lieve Geerts

Co-rapporteurs: -

**Evaluation period:** 

Document status: draft / final

Confidentiality: confidential / restricted / public

#### DOCUMENT HISTORY

Version	Date	Reason of change (responsible person)
1	2016/02/27	Draft_v1
2	2016/04/17	Draft_v2 follow up of discussion of the WCSR during meeting WCSR6
3	2016/05/22	Final version. In the advice the text 'or a similar test using a closed system' was added
4		

## Contents

1 Substance identification	3
2 Concern	4
3 Analysis of available information	4
4 Conclusions	11
5 Advice	12
6 References	12

# 1 Substance identification

Public Name: FC-770

Chemical name: Perfluoro N-alkyl morpholines, C=1,3

EC Number(s): 473-390-7

CAS Number(s): -

Structural formula:



Conclusions of the evaluation	Tick relevant box(es)
Concern not clarified; Need to request further information from the Registrant (s)	Х
Concern clarified; No need of further risk management measures	
Concern clarified; Need for risk management measures;	

## 2 Concern

In the registration dossiers many physical-chemical tests are waived. The main argument from the registrant is that the substance will <u>only</u> be released to air and will NOT deposit from the air compartment. The registrant's claim that FC-770 partitions completely to the air compartment is mainly based on a volatilization study. The concern of the CA is whether this statement is correct.

The request of the CA is: How will FC-770 be distributed in the environment?

- The registrant claims that FC-770 partitions completely to the air compartment, mainly based on a volatilization study. Is this claim reliable? Could the substance be present in condensed state in soil, sediment, and water?
- What is the most reliable model to predict environmental partitioning?
- Can an experimental study of physical-chemical properties deliver reliable results in this respect?

# 3 Analysis of available information

### A. Composition

The substance FC-770 is a mixture of 2 morpholines namely 4-perfluoro-isopropylmorpholine and 4-perfluoro-n-propylmorpholine. The iso-form is the major component.

### B. Physical-chemical properties

An overview of the physical chemical properties is presented in Table 2. The main sources are the CSR (2011) and the EPI Suite models of US-EPA.

### Melting and boiling point

The melting point of FC-770 is -127°C. This key study did not follow an accepted guideline nor was conducted under GLP guidelines. In another study, the melting point was determined to be < -90 °C which supports the key study results. The supporting study followed OECD TG 102, however no method described in OECD TG 102 is considered valid for substances with melting points below - 100 °C.

The boiling point of FC-770 is 96°C at 101.5 kPa. This study was conducted in accordance with OECD TG 103 and is compliant with GLP standards (CSR, 2011). From these experiments it is clear that FC-770 is a liquid at room temperature.

### **Density**

FC-770 is heavier than water. The density of FC-770 is 1.80 g/cm<sup>3</sup> at 20.0 °C. This study was conducted in accordance with OECD TG 109 and is compliant with GLP standards (CSR, 2011).

#### Vapour pressure

The vapor pressure (VP) of FC-770 is 50.6 mm Hg (6.75 kPa) at 20.0 °C. This study satisfies the guideline requirements for test method OECD 104 and is compliant with GLP standards (CSR, 2011). From this high value it is clear that FC-770 is a volatile substance.

For comparison, the measured VP of the volatile perfluorooctane sulfonamide (CAS No. 754-91-6) that is found in ambient air, is 0.25 mm Hg (33.1 Pa) at 20°C (Giesy JP & Kannan K. 2002, referenced in MpBpWIN v. 1.43).

#### Water solubility

The water solubility (WS) of FC-770 is 66.2  $\mu$ g/l at ca. 23 °C. The WS was measured using a scientifically valid method equivalent to OECD TG105 and was conducted under GLP (CSR, 2011). It can be concluded that FC-770 is sparingly soluble in water.

#### <u>Log Kow</u>

Based on the behaviour of some perfluoroalkanes, perfluoroalkyls are expected to form separate layers when mixed with hydrocarbons and water; therefore, measurement of the n-octanol water partition coefficient is not practical (EPA 2005). Therefore the log P was calculated from the solubility ratios in water and alcohol, according to the provisions of OECD TG117. The log Kow at ca. 23 °C is 5.7.

The Log Kow calculated in Kowwin is 4.70 but the reliability of this program for substances of this type is unknown (EA, 2004).

Property	Value	Source
MW	399	CSR, 2011
Physical state	Liquid at room temperature	CSR, 2011
MP	-127°C measured	CSR, 2011
	9.71 °C (n-isomer)	MPBPVP v1.43
BP	96°C measured	CSR, 2011
	55.66 °C (n-isomer)	MPBPVP v1.43
Density	1.80 g/cm <sup>3</sup> measured	CSR, 2011
VP	50,6 mmHg (6.75 kPa) measured at 20°C	CSR, 2011
	44,5 mmHg (5.93 kPa) (n-isomer)	MPBPVP v1.43
WS	66.2 μg/l measured	CSR, 2011
	227.88 µg/l (n-isomer)	WSKOW v1.42
Log Kow	5.7 solubility ratio calculation	CSR, 2011
	(OECD TG 117=HPLC log Kow method)	
	4.70 (n-isomer)	KOWWIN v1.68

Table 2: Physical-chemical and environmental fate properties of FC-770

Henry's law	1030 atm.m <sup>3</sup> /mol = 1,04x105 kPa m <sup>3</sup> /mol, or	CSR, 2011
constant	42400 dimensionless; measured	
	4,07x10 <sup>₄</sup> kPa.m <sup>3</sup> /mol	ECHA, 2016
	0.0134 atm.m <sup>3</sup> /mol or 1.35 kPa-m <sup>3</sup> /mole (n-isomer)	bond method (Henry Win v3.20)
	1.157 atm.m <sup>3</sup> /mol or 117.3 kPa-m <sup>3</sup> /mole (n-isomer)	using user-entered VP and estimated WS (Henry Win v3.20)
Log Koc	4.71 (4.26-5.16) based on log Kow of 5.69 (estimated according TGD chapter 4)	CSR, 2011
	Koc 5.12x10 <sup>4</sup> (EUSES) (log Koc 4.7)	CSR, 2011
	4.341 (MCI method) 3.369 based on Kow (Kow method)	KocWin v2.00
Air-water partition coefficient (Kaw)	1.13x10 <sup>4</sup> , calculated from Henry's law constant (EUSES)	CSR, 2011
Log Koa (octanol-air partitioning)	<ul><li>1.47 is low, so low potential</li><li>Partitioning from air into the lipid rich tissues of air breathing organisms. Calculated from WS and VP</li></ul>	CSR, 2011
Biodegradation	0% after 28 days	CSR, 2011
Hydrolysis	No hydrolysable function	CSR, 2011
Photolysis	Expected lifetime in atmosphere 1500-4000 years	CSR, 2011

### C. Environmental fate properties

An overview of the environmental fate properties is presented in Table 2.

#### **Biodegradation**

The substance is not readily biodegradable. 0% biodegradation was measured after 28 days in sealed vessels. The study was performed according to the OECD TG 310.

#### Hydrolysis

The substance FC-770 has no hydrolysable groups.

#### **Phototransformation**

Degradation in the environment is expected to be by direct photolysis in the upper atmosphere. An additional pathway may be indirect photolysis by singlet atomic oxygen in the stratosphere. An overall lifetime in the range of 1500-4000 years is expected by these processes. The ultimate degradation products are hydrofluoric acid (CAS No. 7664-39-3), water and oxides of nitrogen. These materials are miscible in water and are completely ionised in rainwater. They are expected to undergo wet deposition with no further significant transformation upon return to the troposphere (CSR, 2011).

#### Adsorption/desorption

For most substances, adsorption is predicted on the basis of the log Kow value. As a value for this property cannot be measured for FC-770, this is not possible. Moreover, for surface active substances adsorption or binding behaviour is not triggered by the lipophilicity (i.e. log Kow) (ECHA, 2016). It is not clear whether FC-770 has surface active properties. The test is waived in the registration dossier.

No measurements on the sorption of FC-770 to soils, sediment and sludge are available. The registrant used the values that were calculated using the equation provided in the Technical Guidance Document on Risk Assessment, Chapter 4 "Predominantly hydrophobics". The same equation is applied by EUSES for the calculation of Koc.

PFOS (perfluorooctane sulfonate) is a well-documented perfluorinated compound. In its risk assessment of PFOS, the Environment Agency of the United Kingdom has illustrated that the use of the log Kow for the calculation of Koc in EUSES is not recommended for this substance. To obtain a Koc value in EUSES that was comparable to the Koc calculated from experimental adsorption results, EUSES needed a log Kow of 3.7 (EA, 2004). The log Kow of PFOS is -1,08 (calculated from measured solubility in octanol and water). This means that the adsorption of PFOS is higher than is expected from calculations using the log Kow to calculate Koc in EUSES.

#### **Volatilisation**

The dimensionless Henry's law constant expresses the ratio of vapor phase concentration over aqueous phase concentration. The measured dimensionless Henry's law coefficient of FC-770 is 42400 (volumetric basis) at an average daily temperature of 22 °C. The Henry's Law Constant was determined by measuring the FC-770 concentrations in gas-phase and in aqueous-phase for a given test system vessel at equilibrium conditions and at ambient temperature and pressure. The test was performed according to the equilibrium protocol described in the scientific literature (CSR, 2011). The dimensionless value can be calculated to a Henry's law coefficient of 1030 atm.m<sup>3</sup>/mole or 1.04x10<sup>5</sup> kPa-m<sup>3</sup>/mole at 22°C, using the ideal gas law. The values estimated with HenryWin v3.20 for the n-isomer are orders of magnitude lower: 0.0134 atm.m<sup>3</sup>/mole or 1.35 kPa-m<sup>3</sup>/mole (bond method) without user-entered parameter values for VP and WS, and 1.157 atm.m<sup>3</sup>/mole or 117.3 kPa-m<sup>3</sup>/mole using user-entered VP and estimated WS. The Henry's coefficient calculated with equation R16-4 in the REACH guidance (ECHA, 2016) is 4,07E+04 kPa.m<sup>3</sup>/mol, which is about half of the experimental value.

The Henry's law coefficient is used to describe the tendency for a substance to partition from water to air. The higher the value is, the greater the tendency of the substance to partition from water to air. The measured Henry's law coefficient of FC-770 illustrates that FC-770 is a very volatile substance and will easily evaporate from surface water.

Perfluorooctane sulfonamides (FOSA) and perfluorooctane sulfonamidoethanols (FOSE) are volatile perfluorinated alkyls, and have been detected in ambient air in total mean concentrations of 22-403 pg/m<sup>3</sup> in gas and particulate phase (Canada and USA, 26 samples) and 6-142 pg/m<sup>3</sup> in gas phase (Germany, 11 samples) (Fromme, 2009).

#### Food

No measured data of FC-770 in food items are available. Although perfluorooctane sulfonamides (FOSA) are volatile substances, they have been traced in food. The mean intake of FOSAs and the major metabolite PFOSA, is 59 ng/day (90<sup>th</sup> percentile 280 ng/day) (Tittlemier 2006, referenced by

Fromme, 2009). Substances may end up in crops by direct uptake via soil and indirect via uptake of substances deposited on plant leaves or soil.

According to EUSES the fraction of the total uptake of FC-770 by crops/grass from pore water (8.7E10E-12) is negligible compared to the uptake by crops/grass via air (=1). Likewise, the fraction of the total uptake of FC-770 by cattle from grass is negligible compared to the uptake by cattle via air.

#### Waste water treatment

SimpleTreat is the release model for the waste water treatment plant and is incorporated in EUSES. SimpleTreat assumes that 80% of the wastewater is treated in a biological sewage treatment plant and the remaining 20% released directly into surface waters. SimpleTreat provides release fractions to air, water and sludge as a function of Henry's Law constant and adsorption properties (log Kow or, if available, log Koc) for different biodegradation categories. The distribution of the release of FC-770 was calculated with the log Koc value that was calculated from log Kow. It would be more accurate to perform the calculations with a log Koc that is calculated from measured adsorption/desorption data.

#### Local versus regional releases

The registrant has used EUSES for environmental modelling. As standard assumption 10% of the activity in the region has been used as the basis for the regional emission estimates. Fraction connected to the sewer system is 80%.

In principle, after release to the environment, degradation in the environment and distribution processes should be taken into consideration to estimate the concentrations at the local scale. However, because of the relatively short time between release and exposure, concentrations at local scales are almost entirely controlled by initial mixing (dilution into environmental compartment) and adsorption on suspended matter. Biodegradation may take a role for the soil compartment only. No other process is considered in the calculation of local PECs (ECHA, 2016).

Hence adsorption and biodegradation in the soil are taken into account for the calculation of the local PECs. This underlines the importance of an accurate value for the adsorption/desorption potential.

#### D. Environmental distribution modelling

The environmental distribution of FC-770 is modelled in EUSES and EPIWIN by the registrant. An overview of the results is presented in Table 3.

#### EUSES:

Distribution to environmental compartments (%) from STP release is calculated. The regional scenario from use of FC-770 gives the highest releases (Table 3). For the manufacture scenario no release to STP or water is anticipated. The main release compartment is the ambient air. The calculated fraction of tonnage released to air during manufacture is 0.1%.

However an annual average total deposition flux from air of 0.0365 mg/m<sup>2</sup>/d is calculated, showing that deposition may occur. To which extend the substance is released again to the air or to which extend the deposited substance is adsorbed by plant leaves or to the soil for uptake by plants, is unknown. An accurate measurement of the adsorption/desorption may help to get a better view on the rate of the release/uptake processes.

### EPI Suite

The half-lifes for volatilisation from a river and a lake are two hours and 8 days respectively. After waste water treatment, 47% is adsorbed to the sludge and 43% is released to the ambient air. This is in contradiction with the 0% release calculated in EUSES. EPIWIN includes the Level III Fugacity model of McKay. A Level III model assumes steady-state but not equilibrium conditions. The level III fugacity model in EPI Suite predicts partitioning between air, soil, sediment and water. The main compartments for distribution of FC-770 are soil and sediment. It is not clear whether the Koc used for the distribution is calculated from the log Kow or not.

	FC-770	Model
Local PECs* from	Air: annual average PEC: 0.0216 mg/m <sup>3</sup>	EUSES
manufacture	Air: annual average total deposition flux:	
	0.0365 mg/m <sup>2</sup> /d	
	Surface water: annual local PEC 1.39E-10 mg/l	
	Sediment fresh water: annual local PEC	
	1.55E-7 mg/kg wwt	
	Agricultural soil: annual local PEC 5.32E-6 mg/kg wwt	
Local PECs from	Air: annual average PEC: 1.19E-3 mg/m <sup>3</sup>	EUSES
waste water treatment from manufacture	Air: annual average total deposition flux: 1.66E-5 mg/m²/d	
	Surface water: annual local PEC* 1.39E-10 mg/l	
	Sediment fresh water: annual local PEC 1.55E-7 mg/kg wwt	
	Agricultural soil: annual local PEC 5.32E-6 mg/kg wwt	
Steady-state	Freshwater 1.83E-10 %	EUSES
regional distribution from STP release	Seawater 2.19E-10 %	
during use	Air 0.0159 %	
	Agricultural soil 7.13E-07 %	
	Freshwater sediment 4.25E-09 %	
	Seawater sediment 1.56E-09 %	
Volatilisation from	From river: 2.126 hrs	EPI Suite
water-halflife	From lake: 190.7 hrs (±8 days)	
	Based on Henry's law constant of 0.0134 atm.m <sup>3</sup> /mol	
	n-isomer	
Removal in waste	Total removal 90.3%	EPI Suite
water	Total biodegradation 0.26%	

Table 3: Environmental distribution modelling results

	Total sludge adsorption 47.11%	
	Total to air 42.93%	
	n-isomer	
Level III Fugacity	Air 3.32 %	EPI Suite
model	Water 4.16%	
	Soil 81.6%	
	Sediment 10.9%	
	n-isomer	

\* Predicted environmental concentration

### E. Read across

Read across is the methodology that uses data from one substance to predict the same property for a data-poor substance. A number of perfluoroalkyls, e.g. PFOS and PFOA are well documented regarding those physical-chemical properties that are drivers for their environmental distribution. However their physical-chemical properties are not similar to the properties of FC-770, so read across from these substances for environmental distribution is no option (ECHA, 2013 and EA, 2004).

The registrant uses the substance perfluoro-N-methyl morpholine (PNMM, EC No. 206-841-1, CAS No. 382-28-5) for read across for atmospheric lifetime. Based on structural and spectral similarity, the registrant expects FC-770 and PNMM to have similar atmospheric lifetimes. PNMM differs from FC-770 solely in the alkyl chain(s) attached to the morpholinic nitrogen (CSR, 2011). Another potential substance for read across, proposed by BECA, is perfluamine (EC No. 206-420-2, CAS No. 338-83-0). A comparison of physical-chemical properties of the three substances is presented in Table 4. For the calculation of the Henry's law constant and the air-partitioning coefficient of MNPP and perfluamine, the following equations from the REACH guidance on environmental exposure assessment were used (ECHA, 2016):

$$Henry = \frac{VP.MolW}{Sol}$$
 (Equation R. 16.4)  
$$Kair - water = \frac{Henry}{R.Temp}$$
 (Equation R. 16.5)

With

Henry = Henry's law constant (Pa.m<sup>3</sup>.mol<sup>-1</sup>) K<sub>air-water</sub> = air-water partitioning coefficient (-) VP = vapour pressure (Pa) MolW = molecular weigth (g/mol) Sol = solubility (mg/l) Temp = temperature at the air-water interface = 285°K R = gas constant = 8,314 Pa.m<sup>3</sup>.mol<sup>-1</sup>.K<sup>-1</sup>

Information from the registrant on measured adsorption/desorption or environmental distribution of PNMM or perfluamine is not available to the rapporteur (yet), hence read across to FC-770 is not possible at this moment.

Table 4: Physical-chemical	properties	of perfluoro	morpholines	and perfluamine
Tuble 4.1 Hysical enerniou	properties	or periluoioi	norpriounes	and pointaannine

Property	FC-770 (Source: CSR, 2011)	PNMM (Source: registration dossier*)	Perfluamine (Source: registration dossier*)
MW	399	299	521
Physical state	liquid	liquid	liquid
Density	1.80 g/cm <sup>3</sup>	1.7 g/cm <sup>3</sup>	1.82 g/cm <sup>3</sup>
VP	38 mmHg at 20°C	217.7 mmHg at 20°C	3.87 mmHg at 20°C
	(6.75 kPa)	(29.02 kPa)	(0.516 kPa)
Henry's law	42400 dimensionless	7060 dimensionless	140 000 - 166 000
constant			(category member)
			dimensionless
Air-water	1.13x104 , calculated	4.83x103 (own calculation	2.98x105 (own
partition	from Henry's law	from Henry's law constant	calculation from Henry's
coefficient	constant (EUSES)	with eq. R16.4 and R16.5)	law constant with eq.
(Kaw)			R16.4 and R16.5)
WS	66.2 μg/l	758 µg/l	0.381 µg/l
Log Kow	5.7 solubility ratio	4.3 (shake flask method)	5.3-6.1 (category
	calculation		member)
Adsorption	Adsorption/desorption	Adsorption/desorption	log Koc 5.3 to 6.1 1
	testing is waived	testing is waived	(category member); no
			experimental data
Viscosity	Kinematic viscosity 0.786	Kinematic viscosity 0.5	Kinematic viscosity 0.80
	mm²/s	mm²/s	mm²/s

\* ECHA dissemination website consulted February 2016

## 4 Conclusions

FC-770 is a mixture of perfluorinated morpholines. It is a liquid at room temperature with a vapor pressure of 6.7 kPa at 20°C. FC-770 water solubility is  $66.2\mu g/L$  at 23 °C. Its measured Henry's law constant (expressed as the ratio of vapor phase partial pressure of FC-770 over aqueous phase concentration) is 1030 atm·m<sup>3</sup>/mol at 22 °C. Releases of FC-770 are expected to be to the atmosphere based upon its intended uses. The molecule contains no hydrolysable groups and is not biodegradable. Degradation in the environment is expected to be by mainly by direct photolysis in the upper atmosphere.

The high vapor pressure, low water solubility and the extremely high Henry's law constant combine to move FC-770 from any terrestrial compartment into the atmosphere. The registrant claims that once in the atmospheric compartment, this compound will not partition to terrestrial or aquatic compartments based on the same properties. A calculated value for adsorption/desorption (Koc) is used in the environmental distribution modelling. However it is illustrated for another perfluorinated compound (PFOS) that estimated Koc from log Kow underestimates the adsorption that is seen in measured adsorption/desorption.

Deposition from air to plants and soil are the main sources of FC-770 for crops and animals. There is no data on the extent of re-evaporation to the ambient air form plant surfaces and soil.

Environmental distribution models give diverging results for the contribution of soil/sediment to the distribution. It is unknown to which extend these models take into account the specific chemical behaviour of perfluorinated substances and how large the uncertainties of the predictions are. Finding this out would be interesting from a scientific point of view.

The concern of the BECA on whether the statement of complete partitioning of FC-770 to the air is correct, is regarded to be justified. The registrant claims a complete and swift evaporation of FC-770 from soil after deposition, but provides insufficient data to prove it.

## 5 Advice

4A. Need to request further information from the registrant in order to clarify the concern (concern not clarified)

Measurement of the adsorption/desorption according to OECD TG 106 or a similar test using a closed system. The OECD TG 106 is designed to evaluate the adsorption of a chemical on different soil types with a varying range of organic carbon content, clay content and soil texture, and pH. The measurement should be performed in a closed system. The release to the air should be quantified. The amount that remains in the soil can then be calculated from the mass balance: applied amount minus the evaporated amount. This approach avoids ending up with measured concentrations in the water phase of the soil below the limit of quantification (and no contribution to a solution for the concern). The amount of FC-770 that is not evaporated from the soil should be regarded as bioavailable for soil organisms and plants. It is recognized that this is a worst case approach of the soil (besides solid and water phase), of which the bioavailability for soil organisms and plants is unknown. However, FC-770 is not ready biodegradable and if it remains in the soil, it may stay there for a long time and become a sink. Over time, FC-770 may still become bioavailable in the soil.

Since exposure models give extremely different predictions of the environmental distribution, it is recommended to rely on measurements (as indicated above) to estimate the environmental distribution.

4B. No need for further risk management measurements (concern clarified)

4C. Need for risk management measures (concern clarified)

4D. Others (please specify) 13

### 6 References

CSR, 2011. Chemical Safety Report. Submitted individually. 3M Belgium NV/SA. 2011-07-20

EA, 2004. Environmental risk evaluation report: perfluorooctanesulponate (PFOS). Environment Agency, via <u>https://www.gov.uk/government/organisations/environment-agency</u>

ECHA, 2013. Substance Name: Pentadecafluorooctanoic Acid (PFOA) EC Number: 206-397-9 CAS Number: 335-67-1. Member State Committee support document for identification of pentadecafluorooctanoic acid (PFOA) as a substance of very high concern because of its CMR and PBT properties. Adopted on 14 June 2013

ECHA, 2016. Guidance on information requirements and chemical safety assessment. Chapter R.16: Environmental exposure assessment

EPA. 2005. Draft risk assessment of the potential human health effects associated with exposure to perfluorooctanoic acid and its salts. U.S. Environmental Protection Agency. http://www.epa.gov/opptintr/pfoa/pubs/pfoarisk.pdf. June 26, 2007.

Fromme, H.; Tittlemier, S. A.; Volkel, W.; Wilhelm, M.; Twardella, D. 2009. Perfluorinated compounds - Exposure assessment for the general population in western countries Int. J. Hyg. Environ. Health 2009, 212 (3) 239–270