ANNEX A: PFOS_FLUOREX_AUG2025 SUBSTANCE SHEET

Parameter	Unit	Value	Source
Name		Perfluorooctane sulfonic acid	
CAS number EC number		1763-23-1 217-179-8	
Type		organic	
Dissociative		no[(1)]	
Acid constant (pKa)		-3.27	Brooke *et al.* (2004)
Molar mass	g/mol	500.126	
Water solubility	mg/l	370 (K-salt)[(2)]	OECD (2002), freshwater, 20°C assumed
Vapour pressure	Pa	3.31×10^{-4} (K-salt) (20°C)	OECD (2002)
Henry coefficient	Pa m³/mol	-	Calculated in S-Risk
Log K_{ow}[1] K_{ow}	g/g	4.49 (calculated value)[(3)] 30902.95	EpiSuite
Log K_{oc} K_{oc}	dm³/kg	2.57 (anion) 371.54	Higgins and Luthy (2006)
Log K_{oa}	g/g	-[(4)]	Optional in S-Risk
BCF	(mg/kg dm)/(mg/m³)	See table below	
Dpe	m²/d	1×10^{-7} (standard value)	Based on Vonk (1985) and Lijzen *et al.* (2011)
Dpvc	m²/d	1×10^{-10} (Dpe/1000)	Cornelis *et al.* (2017)
Diffusion for organic substance in air (Da)	m²/d	-	Calculated in S-Risk
Diffusion for organic substance in water (Dw)	m²/d	-	Calculated in S-Risk
Kp	[cm/h]	9.5×10^{-7} (AFPO)	Washburn *et al.* (2005)
FA	-	1	Cornelis *et al.* (2017)
ABS dermal soil/dust	-	0	Xiao *et al.* (2015)

[1] Entered in S-Risk but not used in further calculations

Parameter	Unit	Value	Source
BTF beef	d/kg	0.071	Vestergren *et al.* (2013)
BTF sheepmeat	d/kg	0.387	Kowalczyk *et al*. (2012)
BTF liver	d/kg	0.441	Vestergren *et al.* (2013)
BTF kidney	d/kg	1.201	Kowalczyk *et al.* (2013)
BTF milk	d/kg	0.021	Vestergren *et al.* (2013)
BTF soil – egg	d/kg		
BTF food - egg	d/kg		
Carcinogenicity		Carc. 2	EG (2008)
Systemic effects threshold			
TDI oral	mg/kg.d	6.3×10^{-7}	EFSA 2020
TCA inhalatory	[mg/m³]	2.21×10^{-6}	calculated from TDI oral
TDI dermal	mg/kg.d	6.3×10^{-7}	= TDI oral
smoothing - ages		Adult	
Limit in air	mg/m³	-	
Limit in drinking water	mg/m³	0.1	EC (2018)
Crop standard	mg/kg fw		
Meat and edible offal standard			EU (2022) [2]
Beef	mg/kg fw	3×10^{-4}	
Sheepmeat	mg/kg fw	1×10^{-3}	
Liver	mg/kg fw	6×10^{-3}	
Kidney	mg/kg fw	6×10^{-3}	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	1×10^{-3}	
Dietary background all age groups including children	mg/kg day	5.32×10^{-8} (1 - < 3 y)	FLUOREX data LB(5)
		8.43×10^{-8} (3 - < 6 y)	
		6.43×10^{-8} (6 - < 10 y)	
		5.57×10^{-8} (10 - < 15 y)	
		5.14×10^{-8} (15 - < 21 y)	
		5.14×10^{-8} (21 - < 31 y)	
		5.57×10^{-8} (31 - < 61 y)	
		6.29×10^{-8} (≥ 61 y)	
Background potato	mg/kg fw	0	FLUOREX data LB
Background root vegetables	mg/kg fw	0	FLUOREX data LB

[2] Publications Office (europa.eu)

Parameter	Unit	Value	Source
Background bulbous vegetables (onion, etc.)	mg/kg fw	0	FLUOREX data LB
Background fruiting vegetables	mg/kg fw	0	FLUOREX data LB
Background cabbage	mg/kg fw	0	FLUOREX data LB
Background leafy vegetables	mg/kg fw	7.20×10^{-8}	FLUOREX data LB
Background legumes	mg/kg fw	0	FLUOREX data LB
Background beef	mg/kg fw	2.4×10^{-5}	FLUOREX data LB
Background offal	mg/kg fw	1.05×10^{-4}	FLUOREX data LB
Background milk	mg/kg fw	0	FLUOREX data LB
Background butter	mg/kg fw	0	FLUOREX data LB
Background eggs	mg/kg fw	0	FLUOREX data LB
Background outdoor air	mg/m³	1.4×10^{-9}	P50 value from Cornelis *et al.* (2009)
Background indoor air	mg/m³	1.6×10^{-9}	Jahnke *et al.* (2007b) in Cornelis *et al.* (2009)
Background drinking water	mg/m³	0	Assimilated to zero since it is included in the intake estimation of FLUOREX

(1) in S-Risk 'no' is entered because the Kd of dissociative substances is calculated from log K_{ow}, which we want to avoid; for non-dissociative substances the Kd is calculated from the K_{oc}

(2) The value of 370 mg/l is given in OECD (2002) with reference to a 3M report from 1999, without mention of temperature. The OECD test protocol for solubility (OECD test guideline 105) states that the test should preferably be carried out at 20 ± 0.5°C. As such, 20°C is used in S-Risk.

(3) Log K_{ow} is mandatory in S-Risk, and is used to calculate Kp, K_{oc}, and transfer factors, unless an experimental value is entered. Experimental values are available for these three parameters.

(4) Log K_{oa} is optional in S-Risk, which uses K_{oa} in the calculation of transfer to plants; as experimental data are available for this purpose, a K_{oa} value is not necessary.

(5) The exposure data used in the estimation were obtained from the FLUOREX project (RF 21/6350), realized by Sciensano and funded by the Belgian Federal Public Service Health, Food Chain Safety and Environment.

Plant	BCF or BCF model
potatoes	
potatoes	**0.01**
root and tuber vegetables	
carrots	**0.50**
salsify	0.44 (= average known root and tuber vegetables)
other root vegetables (such as radish)	**0.38**
bulbous vegetables	
bulbous vegetables (such as onion)	0.44 (= average known root and tuber vegetables)
leek	0.44 (= average known root and tuber vegetables)
fruiting vegetables	
tomato	**0.06**
cucumber	**0.07**
other fruiting vegetables (such as peppers)	0.065 (average known fruiting vegetables)
cabbages	
cabbage	0.44 (= average known root and tuber vegetables)
cauliflower and broccoli	0.44 (= average known root and tuber vegetables)
sprouts	0.44 (= average known root and tuber vegetables)
leafy vegetables	
lettuce	**0.56**
lamb's lettuce	0.56 (= lettuce)
endive	0.62 (average lettuce and celery)
spinach	**3.77**
chicory	0.62 (average lettuce and celery)
celery	**0.72**
legumes	
beans	0.03 (= peas)
peas	**0.03**
grasses	
grass	**0.048**
cereals	
maize	**0.003**

ANNEX B: PFOA_FLUOREX_AUG2025 SUBSTANCE SHEET

Parameter	Unit	Value	Source
Name		Perfluorooctanoic acid	
CAS number EC number		335-67-1 206-397-9	
Type		organic	
Dissociative		no[1]	
Acid constant (pKa)		2.8	Moody and Field (2000)
Molar mass	g/mol	414.07	
Water solubility	mg/l	9.5×10^{3} (25°C)	ECHA (2014)
Vapour pressure	Pa	1.7×10^{-2} (10°C)	Lijzen *et al.* (2018)
Henry coefficient	Pa m³/mol	-	Calculated in S-Risk
Log K_{ow}[3] K_{ow}	g/g	4.81 (calculated value)[2] 64565.42	EpiSuite
Log K_{oc} K_{oc}	dm³/kg	2.06 114.82	Higgins and Luthy (2006)
Log K_{oa}	g/g	-[3]	optional in S-Risk
BCF	(mg/kg dm)/(mg/m³)	See table below	
Dpe	m²/d	1×10^{-7} (standard value)	Vonk (1985); Lijzen *et al.* (2018)
Dpvc	m²/d	1×10^{-10} (Dpe/1000)	Cornelis *et al.* (2017)
Diffusion for organic substance in air (Da)	m²/d	-	Calculated in S-Risk
Diffusion for organic substance in water (Dw)	m²/d	-	Calculated in S-Risk
Kp	[cm/h]	9.49×10^{-7}	Fasano *et al.* (2005)
FA	-	1	Cornelis *et al.* (2017)
ABS dermal soil/dust	-	0	Xiao *et al.* (2015)
BTF beef	d/kg	5.999×10^{-3}	Vestergren, 2013 and Kowalczyk *et al.* (2013)

[3] Entered in S-Risk but not used in further calculations

Parameter	Unit	Value	Source
BTF sheepmeat	d/kg	6.950×10^{-3}	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF liver	d/kg	8.756×10^{-3}	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF kidney	d/kg	1.945×10^{-3}	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF milk	d/kg	5.686×10^{-3}	Vestergren, 2013 and Kowalczyk *et al.* (2013)
BTF soil – egg	d/kg		
BTF food - egg	d/kg		
Carcinogenicity		Carc. 2	EC (2008)
Systemic effects threshold [4]			
TDI oral	mg/kg.d	6.3×10^{-7}	EFSA 2020 for PFOS + PFOA + PFNA + PFHxS, fully attributed to PFOS
TCA inhalatory	mg/m³	2.21×10^{-6}	calculated from TDI oral
TDI dermal	mg/kg.d	6.3×10^{-7}	= TDI oral
smoothing - ages		adult	
Systemic effects without threshold			
Slope factor oral	$(mg/kg/d)^{-1}$	0.07[5]	US-EPA (2016d)
Unit risk	$(mg/m^3)^{-1}$	-	
Slope factor dermal	$(mg/kg/d)^{-1}$	-	
Smoothing duration		Adult	
Limit in air	mg/m³	-	
Limit in drinking water	mg/m³	0.1	EC (2018)
Crop standard	mg/kg fw		
Meat and edible offal standard			EU (2022) [4]
Beef	mg/kg fw	8×10^{-4}	
Sheepmeat	mg/kg fw	2×10^{-4}	
Liver	mg/kg fw	7×10^{-4}	
Kidney	mg/kg fw	7×10^{-4}	
Milk	mg/kg fw	-	

[4] Publications Office (europa.eu)

Parameter	Unit	Value	Source
Butter	mg/kg fw	-	
Egg	mg/kg fw	3×10^{-4}	
Dietary background all age groups including children	mg/kg day	1.03×10^{-7} (1 - < 3 y)	FLUOREX data LB[(5)]
		1.63×10^{-7} (3 - < 6 y)	
		9.71×10^{-8} (6 - < 10 y)	
		7.71×10^{-8} (10 - < 15 y)	
		6.71×10^{-8} (15 - < 21 y)	
		6.14×10^{-8} (21 - < 31 y)	
		5.71×10^{-8} (31 - < 61 y)	
		5.57×10^{-8} (≥ 61 y)	
Background potato	mg/kg fw	0	FLUOREX data LB
Background root vegetables	mg/kg fw	5.30×10^{-6}	FLUOREX data LB
Background bulbous vegetables (onion, etc.)	mg/kg fw	6.97×10^{-6}	FLUOREX data LB
Background fruiting vegetables	mg/kg fw	1.10×10^{-5}	FLUOREX data LB
Background cabbage	mg/kg fw	1.20×10^{-5}	FLUOREX data LB
Background leafy vegetables	mg/kg fw	1.34×10^{-5}	FLUOREX data LB
Background legumes	mg/kg fw	4.30×10^{-6}	FLUOREX data LB
Background beef	mg/kg fw	1.60×10^{-5}	FLUOREX data LB
Background offal	mg/kg fw	0	FLUOREX data LB
Background milk	mg/kg fw	0	FLUOREX data LB
Background butter	mg/kg fw	0	FLUOREX data LB
Background eggs	mg/kg fw	0	FLUOREX data LB
Background outdoor air	mg/m³	8.90×10^{-9}	Cornelis *et al.* (2009)
Background indoor air	mg/m³	$8.90\times.10^{-9}$	Assimilated to outdoor air
Background drinking water	mg/m³	0	Assimilated to 0 since it is included in the intake estimation FLUOREX

[(1)] in S-Risk 'no' is entered because the Kd of dissociative substances is calculated from log K_{ow}, which we want to avoid; for non-dissociative substances the Kd is calculated from the K_{oc}

(2) Log K_{ow} is mandatory in S-Risk, and is used to calculate Kp, K_{oc}, and transfer factors, unless an experimental value is entered. Experimental values are available for these three parameters.
(3) Log K_{oa} is optional in S-Risk, which uses K_{oa} in the calculation of transfer to plants; as experimental data are available for this purpose, a K_{oa} value is not necessary.
(4) The slope factor corresponds with a dose of $1.43.10^{-4}$ mg/kg bw/d or 143 ng/kg bw/d for an additional cancer risk of $1/10^5$. This value is higher than the toxicological reference value (20 ng/kg bw/d) used for the derivation of the soil remediation values. Hence a soil remediation value based on carcinogenic effects was not derived as it could be expected to be higher than for non-carcinogenic effects. This statement is in line with US-EPA who confirmed that the lifetime health advisory (2.10^{-5} mg/kg bw/d) based on non-cancer effects is protective for the cancer endpoint (US-EPA, 2016b).
(5) The exposure data used in the estimation were obtained from the FLUOREX project (RF 21/6350), realized by Sciensano and funded by the Belgian Federal Public Service Health, Food Chain Safety and Environment.

BCF values PFOA

Plant	BCF or BCF model
potatoes	
potatoes	**0.06**
root and tuber vegetables	
carrots	**0.39**
salsify	0.55 (average value of known root and tuber vegetables)
other root vegetables (such as radish)	**0.70**
bulbous vegetables	
bulbous vegetables (such as onion)	0.55 (= average known root and tuber vegetables)
leek	0.55 (= average known root and tuber vegetables)
fruiting vegetables	
tomato	**0.81**
cucumber	**0.82**
other fruiting vegetables (such as peppers)	0.81 (=tomato)
Cabbages	
Cabbage	0.55 (= average known root and tuber vegetables)
cauliflower and broccoli	0.55 (= average known root and tuber vegetables)
sprouts	0.55 (= average known root and tuber vegetables)
leafy vegetables	
Lettuce	**1.90**
lamb's lettuce	1.90 (= lettuce)

Plant	BCF or BCF model
endive	1.06 (= average of all known leafy vegetables)
spinach	**0.87**
chicory	1.06 (= average of all known leafy vegetables)
celery	**0.42**
legumes	
beans	0.03 (= peas)
peas	**0.03**
Grasses	
Grass	**0.128**
Cereals	
Maize	**0.005**