

S-Risk for the Walloon region - substance datasheet: PFOA, PFOS and PFDA

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List of acronyms

ABS	Absorption factor
Al	Aluminum content
BCF	Bioconcentration factor
BTF	Biotransfer factor
Da	Diffusion coefficient in air
Dpe	Diffusion coefficient in polyethylene
Dpvc	Diffusion coefficient in PVC
Dw	Diffusion coefficient in water
FA	Factor used when calculating dermal absorption from water
Fe	Iron content
ISSeP	Institut Scientifique de Service Public
K _d	Sorption coefficient soil-water
K _{oa}	Distribution coefficient octanol-air
K _{oc}	Distribution coefficient organic carbon-water
K _{ow}	Distribution coefficient octanol-water
K _p	Dermale permeability coefficient
PAH	polycyclic aromatic hydrocarbons
P _{tot}	Total phosphorus content
TCA	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TGD	Technical Guidance Document

Introduction

As knowledge about environmental behaviour and toxicity of PFAS is moving fast, the chemicals encoded in S-RISK® WAL are indicated with the date, correlated with the date of the enforcement of the "Guidelines for PFAS" in Wallonia.

This specification allows to add these chemicals with updated data further without deleting the previous ones.

Due to surfactant properties of PFAS, some parameters are difficult to measure experimentally:

- the octanol-water coefficient **Kow** cannot be measured using current OECD methods. Kow is mandatory in S-Risk and has to be filled in anyway. For this, it can be calculated by EpiSuite even if EpiSuite is not recommended. To avoid using the Kow value in equations (equations to calculate Kp, Koc, BioConcentration Factors (BCF) and BioTransfer Factors (BTF)), **data of Kp, Koc, BCF and BTF must be encoded to obtain a correct result of risk**. The algorithms currently used for BCF and BTF (Trapp, Travis & Arms) are not applicable. Kow is entered in S-Risk but has not to be used in further calculations.
- the Henry constant **H** must be calculated by S-Risk, based on the vapour pressure and the solubility instead of encoding an experimental value.
- the PFAS are considered "**no dissociative**" because the Kd of dissociative substances is calculated from log Kow, which we want to avoid; for non-dissociative substances the Kd is calculated from the Koc.

For PFAS, some specificities are already taken account in the algorithm of the S-Risk® model core and need a specific key to consider them as PFAS. **All chemicals with a name starting by the 4 first letters "PFOA", "PFOS" or "PFAS" will be considered as a PFAS for the calculation**. It allows S-Risk to calculate the ingestion of vegetables with BioConcentration Factors (BCF) for soil/plant transfer expressed in different units.

As explained previously, BCF for soil/plant transfer must be encoded if the ingestion of vegetables pathway is selected (e.g. residential and agricultural exposure scenarios). As the transfer of PFAS is linked to the soil concentration, the experimental BCF are expressed in scientific literature with different units: **(mg/kg plant dm)/(mg/kg soil dm)** instead of (mg/kg dm)/(mg/m³) for classic chemicals.

PFOA and PFOS_dec2023

The data used to calculate the limit values in soil for PFOA and PFOS in S-Risk® WAL were selected:

- in **February 2020** for toxicity data by SPAQUE and ISSeP,
- updated in **December 2023** for chemical parameters, BCF and BTF, thanks to the huge scientific review of the literature done by VITO (2020). That means that chemical parameters, BCF and BTF all come from VITO (2020) and are exactly the same in S-RISK® WAL and in S-RISK® VLA/BXL.

But the toxicity data have not yet been updated since February 2020: the update of Toxicity Reference Values by EFSA in 2020 and the update of the carcinogenic effects by « The Lancet Oncology » in November 2023 are not taken account in the risk assessment.

Reference : M. Van Holderbeke, J. Bierkens, L. Geerts. Proposal for soil remediation values for Perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA). Study carried out on behalf of OVAM. 2019/Unit/R/2055. October 2020.

In order to follow the principle of transparency and to find the data origins, the references coming from VITO report (VITO, 2020) are indicated in the reference column.

PFDA_dec2023

The data used to calculate the limit values in soil for PFDA were selected in **March 2023** for all parameters. The methodology used for the selection of BCF and BTF was similar as for PFOA and PFOS by VITO (2020).

Experimental studies show the following relationship in the soil/plant transfer: in general, the BCF for multiple vegetables present a linear decrease trend with increasing carbon chain length, considering a distinction between carboxylic and sulfonic.

Following this assumption and the precaution principle, if BCF data for PFDA (C10) was not available for a given vegetable, data of PFOA (C8) for this vegetable were selected, considering PFOA as the nearer carboxylic PFAS.

PFDA_dec2024

In **December 2024**, the Vapour Pressure V_p was modified and corrected with the pK_a , following the Lijzen formula (Lijzen, 2018). The Henry constant, calculated from V_p , M and S was also corrected.

PFOA-dec2023

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	Perfluorooctanoic acid	Pubchem
Name S-Risk WAL	-	PFOA-dec2023	
Molecular formula		C ₈ HF ₁₅ O ₂	Pubchem
CAS number	-	335-67-1	Pubchem
EC number	-	206-397-9	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	Acid	
Acid constant - pKa		2,8	Moody and Field (2000)
Molar mass - M	g/mol	414,07	Pubchem
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	9500	ECHA (2014)
Temperature for P - Tp	°C	10	
Vapour pressure - Pa	Pa	1,7.10 ⁻²	Lijzen et al. (2018)
Temperature for Henry coefficient - Th	°C	10	
Henry coefficient - H	Pa.m ³ /mol	7,41.10 ⁻⁴	Calculated from H = (P x M) / S
Organic carbon-water partition coefficient - Koc	dm ³ /kg	114,82	Higgins and Luthy (2006)
Log Koc		2,06	
Octanol-water partition coefficient - Kow	-	64565,42	EpiSuite
Log Kow		4,81	
Permeation organic substance through PE pipe - Dpe	m ² /d	1.10 ⁻⁷	Vonk (1985) Lijzen et al. (2018)
Permeation organic substance through PVC pipe - Dpvc	m ² /d	(1.10 ⁻¹⁰)	Calculated by S-Risk
Soil-water distribution coefficient Kd	l/kg	Not relevant	
Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	9,49.10 ⁻⁷	Fasano et al. (2005)

Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0	Xiao et al. (2015)
Fraction absorbed water - FA	-	0,2	Cornelis et al. (2017)

Plant	BCF plant	Source
Potatoes		
Potatoes	0,06	Average values Lechner et al. (2011)
Root and tuber vegetables		
Carrots	0,39	Average value Lechner and Knapp (2011) and Bizkarguenaga et al. (2016)
Salsify	0,55	Average value of known root and tuber vegetables
Other root vegetables (such as radish)	0,70	Average values Blaine et al. (2014)
Bulbous vegetables		
Bulbous vegetables (such as onion)	0,55	Average value of known root and tuber vegetables
Leek	0,55	Average value of known root and tuber vegetables
Fruiting vegetables		
Tomato	0,81	Single value Blaine et al. (2013) and Blaine et al. (2014)
Cucumber	0,82	Average values from Lechner et al. (2011)
Other fruiting vegetables (such as peppers)	0,81	= tomato BCF
Cabbages		
Cabbage	0,55	Average value of known root and tuber vegetables
Cauliflower and broccoli	0,55	Average value of known root and tuber vegetables
Sprouts	0,55	Average value of known root and tuber vegetables
Leafy vegetables		
Lettuce	1,90	Average value Blaine et al. (2013) and Bizkarguenaga et al. (2016)
Lamb's lettuce	1,90	= lettuce BCF
Endive	1,06	Average of all known leafy vegetables
Spinach	0,87	Single value Navarro et al. (2017)
Chicory	1,06	Average of all known leafy vegetables
Celery	0,42	Average values Blaine et al. (2014)
Legumes		
Beans	0,03	= peas BCF
Peas	0,03	Single value Blaine et al. (2014)
Grasses		

Grass	0,128	Average value Stahl et al. (2009)
Cereals		
maize	0,005	Single value Stahl et al. (2009)

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)	$5,999.10^{-3}$	Vestergren et al. (2013) and Kowalczyk et al. (2013)
Cow liver BTF	(mg/kg fw)/(mg/d)	$8,756.10^{-3}$	Vestergren et al. (2013) and Kowalczyk et al. (2013)
Cow kidney BTF	(mg/kg fw)/(mg/d)	$1,945.10^{-3}$	Vestergren et al. (2013) and Kowalczyk et al. (2013)
Cow milk BTF	(mg/kg fw)/(mg/d)	$5,686.10^{-3}$	Vestergren et al. (2013) and Kowalczyk et al. (2013)
Sheep meat BTF	(mg/kg fw)/(mg/d)	$6,950.10^{-3}$	Vestergren et al. (2013) and Kowalczyk et al. (2013)
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)		
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)		

Limit value	Unit	Value	Source
Drinking water	$\mu\text{g/l}$		
Outdoor air	mg/m^3		
Indoor air	mg/m^3		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m^3	$1,190.10^{-5}$	Derivation from the occupational exposure limit value (VLEP) (for example TCEQ 5.10^{-6} mg/m^3)
TDI oral	$\text{mg}/(\text{kg}\cdot\text{d})$	3.10^{-6}	ATSDR (2018)
TDI dermal	$\text{mg}/(\text{kg}\cdot\text{d})$	3.10^{-6}	= TDI oral
Systemic effects non-threshold			
Unit risk for inhalation	$(\text{mg}/\text{m}^3)^{-1}$	2.10^{-2}	Derivation oral route → inhalation route
Oral slope factor	$(\text{mg}/\text{kg}\cdot\text{d})^{-1}$	7.10^{-2}	US-EPA (2016)
Dermal slope factor	$(\text{mg}/\text{kg}\cdot\text{d})^{-1}$	7.10^{-2}	= TDI oral

PFOS-dec2023

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	Perfluorooctane sulfonic acid	Pubchem
Name S-Risk WAL	-	PFOS-dec2023	
Molecular formula		C ₈ F ₁₇ SO ₃ H	Pubchem
CAS number	-	1763-23-1	Pubchem
EC number	-	217-179-8	Pubchem
Organic	-	Yes	
Dissociating	-	No	
Type Acid/Base	-	Acid	
Acid constant - pKa		-3,27	Brooke et al. (2004)
Molar mass - M	g/mol	500,126	Pubchem
Temperature for water solubility - Ts	°C	20	
Water solubility - S	mg/l	370	OECD (2002) ¹
Temperature for P - Tp	°C	20	
Vapour pressure - Pa	Pa	3,31.10 ⁻⁴	OECD (2002)
Temperature for Henry coefficient - Th	°C	20	
Henry coefficient - H	Pa.m ³ /mol	4,474.10 ⁻⁴	Calculated from H = (P x M) / S
Organic carbon-water partition coefficient - Koc	dm ³ /kg	371,54	Higgins and Luthy (2006) - anion
Log Koc		2,57	
Octanol-water partition coefficient - Kow	-	30902,95	Calculated by EpiSuite
Log Kow		4,49	
Permeation organic substance through PE pipe - Dpe	m ² /d	1.10 ⁻⁷	Vonk (1985) Lijzen et al. (2011)
Permeation organic substance through PVC pipe - Dpvc	m ² /d	(1.10 ⁻¹⁰)	Calculated by S-Risk
Kd	l/kg	Not relevant	

¹ 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.

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h	$9,5 \cdot 10^{-7}$	Washburn et al. (2005)
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0	Xiao et al. (2015)
Fraction absorbed water - FA	-	0,2	Cornelis at al. (2017)

Plant	BCF plant	Source
Potatoes		
Potatoes	0,01	Single value Lechner and Knapp (2011)
Root and tuber vegetables		
Carrots	0,50	Average value Lechner and Knapp (2011) and Bizkarguenaga et al. (2016)
Salsify	0,44	Average known root and tuber vegetables
Other root vegetables (such as radish)	0,38	Average values Blaine et al. (2014)
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	Single value Navarro et al. (2017)
Cucumber	0,07	Single value from Lechner and Knapp (2011)
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	Average value Blaine et al. (2013) and Bizkarguenaga et al. (2016)
Lamb's lettuce	0,56	= lettuce BCF
Endive	0,62	Average of lettuce and celery
Spinach	3,77	Average values Navarro et al. (2017)
Chicory	0,62	Average of lettuce and celery
Celery	0,72	Average values Blaine et al. (2014)
Legumes		
Beans	0,03	= peas BCF
Peas	0,03	Single value Blaine et al. (2014)

Grasses		
Grass	0,048	Lowest value Stahl et al. (2009)
Cereals		
maize	0,003	Single value Stahl et al. (2009)

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)	0,071	Vestergren et al. (2013)
Cow liver BTF	(mg/kg fw)/(mg/d)	0,441	Vestergren et al. (2013)
Cow kidney BTF	(mg/kg fw)/(mg/d)	1,201	Kowalczyk et al. (2013)
Cow milk BTF	(mg/kg fw)/(mg/d)	0,021	Vestergren et al. (2013)
Sheep meat BTF	(mg/kg fw)/(mg/d)	0,387	Kowalczyk et al. (2012)
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)		
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)		

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³		
Indoor air	mg/m ³		

Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	2,380.10 ⁻⁵	Derivation from the occupational exposure limit value (VLEP) (for example TCEQ 1.10 ⁻⁵ mg/m ³)
TDI oral	mg/(kg.d)	2.10 ⁻⁶	ATSDR (2018)
TDI dermal	mg/(kg.d)	2.10 ⁻⁶	= TDI oral
Systemic effects non-threshold			
Unit risk for inhalation	(mg/m ³) ⁻¹	2.10 ⁻²	Derivation oral route → inhalation route (PFOA)
Oral slope factor	(mg/kg.d) ⁻¹	7.10 ⁻²	US-EPA (2016) (PFOA)

Dermal slope factor	$(\text{mg}/\text{kg}\cdot\text{d})^{-1}$	$7\cdot 10^{-2}$	= TDI oral
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PFAS_PFDA_dec2023

PFAS PFDA dec2024

Physico-chemical parameter	Unit	Value	Source
Name (complete)	-	Perfluorodecanoic acid	Pubchem
Name S-Risk WAL	-	PFAS_PFDA_dec2023	
<u>Name S-Risk WAL</u>	-	<u>PFAS PFDA dec2024</u>	
Molecular formula		C ₉ F ₁₉ COOH	Pubchem
CAS number	-	335-76-2	Pubchem
EC number	-	206-400-3	Pubchem
Organic	-	Yes	
Dissociating	-	No	pKa < 2 = always under ionic form
Type Acid/Base	-		
Acid constant - pKa			
Molar mass - M	g/mol	514,08	Pubchem
Temperature for water solubility - Ts	°C	25	
Water solubility - S	mg/l	5,14.10 ³	Kauch & Diesslin (1951) in ECHA et ITRC (max. exp)
Temperature for P - Tp	°C	25	
Vapour pressure - Pa	Pa	1.10 ⁻¹	Pubchem + ATDSR
<u>Vapour pressure - Pa</u>	<u>Pa</u>	<u>1,044.10⁻⁶</u>	<u>Pubchem + ATDSR</u> <u>Correction with pKa</u> <u>pKa = 0 (values</u> <u>between -0.17 and</u> <u>0.4)</u>
Temperature for Henry coefficient - Th	°C	25	
Henry coefficient - H	Pa.m ³ /mol	1,00015.10 ⁻²	Calculated from H = (P x M) / S
<u>Henry coefficient - H</u>	<u>Pa.m³/mol</u>	<u>1,044.10⁻⁷</u>	<u>Calculated from H =</u> <u>(P x M) / S</u>
Organic carbon-water partition coefficient - Koc	dm ³ /kg	616	ATSDR
Log Koc		2,79	

Octanol-water partition coefficient - Kow	-	3,16.10 ⁶	Calculated by EpiSuite
Log Kow		6,49	
Permeation organic substance through PE pipe - Dpe	m ² /d	0	Lijzen et al. (2001)
Permeation organic substance through PVC pipe - Dpvc	m ² /d	0	
Kd	l/kg	Not relevant	

Exposure parameter	Unit	Value	Source
Dermal permeability coefficient - Kp	cm/h		Use model
Dermal absorption factor for soil and dust - ABS dermal soil/dust	-	0,25	
Fraction absorbed water - FA	-	0,2	Cornelis at al. (2017)

Plant	BCF plant	Source
Potatoes		
Potatoes	0,06	Value for PFOA (worst case) – no specific experimental data on PFDA in potatoes <i>Lechner (2011)</i>
Root and tuber vegetables		
Carrots	0,47	Value for radish
Salsify	0,47	Value for radish
Other root vegetables (such as radish)	0,47	Maximal value from 2 available values in Blaine et al. (2014)
Bulbous vegetables		
Bulbous vegetables (such as onion)	0,77	Liu (2019)
Leek	0,77	Value for onion
Fruiting vegetables		
Tomato	0,02	Navarro et al. (2017) Values < LOQ in Blaine (2013)
Cucumber	0,02	Value for tomato
Other fruiting vegetables (such as peppers)	0,02	Value for tomato
Cabbages		
Cabbage	0,55	Value for PFOA (worst case)
Cauliflower and broccoli	0,55	Value for PFOA (worst case)
Sprouts	0,55	Value for PFOA (worst case)

Leafy vegetables		
Lettuce	0,52	Maximal value from 2 available values in Blaine et al. (2013)
Lamb's lettuce	0,52	Value for lettuce
Endive	0,52	Value for lettuce
Spinach	0,52	Value for lettuce
Chicory	0,52	Value for lettuce
Celery	0,32	Maximal value from 2 available values in Blaine et al. (2014)
Legumes		
Beans	0,03	Value for PFOA (worst case) <i>Blaine (2014)</i>
Peas	0,03	Value for PFOA (worst case) <i>Blaine (2014)</i> In Blaine (2014), concentration < LOQ for peas
Grasses		
Grass	0,128	Value for PFOA (worst case) <i>Stahl et al. (2009)</i>
Cereals		
maize	0,04	Krippner (2015)

Animal parameter	Unit	Value	Source
Cow meat BTF	(mg/kg fw)/(mg/d)	$2,450 \cdot 10^{-2}$	Vestergren et al. (2013)
Cow liver BTF	(mg/kg fw)/(mg/d)	$2,179 \cdot 10^{-1}$	Vestergren et al. (2013)
Cow kidney BTF	(mg/kg fw)/(mg/d)	$9,880 \cdot 10^{-2}$	Calcul use model
Cow milk BTF	(mg/kg fw)/(mg/d)	$1,659 \cdot 10^{-2}$	Vestergren et al. (2013)
Sheep meat BTF	(mg/kg fw)/(mg/d)	$9,880 \cdot 10^{-2}$	Calcul use model
Chicken - soil to egg BTF	(mg/kg fw)/(mg/d)		
Chicken - feed to egg BTF	(mg/kg fw)/(mg/d)		

Limit value	Unit	Value	Source
Drinking water	µg/l		
Outdoor air	mg/m ³		

Indoor air	mg/m ³		
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Toxicological Reference value	Unit	Value	Source
Systemic effects threshold			
TCA inhalatory	mg/m ³	9,10.10 ⁻⁴	Derivation oral route → inhalation route
TDI oral	mg/(kg.d)	2,60.10 ⁻⁴	Calculation done by SPAQuE (2023) on basis of Harris and Birnbaum (1989)
TDI dermal	mg/(kg.d)	2,60.10 ⁻⁴	= TDI oral
Systemic effects non-threshold			
Unit risk for inhalation	(mg/m ³) ⁻¹	41	Derivation oral route → inhalation route
Oral slope factor	(mg/kg.d) ⁻¹	143	OEHHA (2019) for PFOA
Dermal slope factor	(mg/kg.d) ⁻¹	143	= TDI oral

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