

## ANNEX A: PFOS EFSA 2020 SUBSTANCE SHEET

Parameter	Unit	Value	Source
Name		Perfluorooctane sulfonic acid	
CAS number		1763-23-1	
EC number		217-179-8	
Type		organic	
Dissociative		no <sup>(1)</sup>	
Acid constant (pKa)		-3.27	Brooke <i>et al.</i> (2004)
Molar mass	g/mol	500,126	
Water solubility	mg/l	370 (K-salt) <sup>(2)</sup>	OECD (2002)
Vapour pressure	Pa	3.31.10 <sup>-4</sup> (K-salt) (20°C)	OECD (2002)
Henry coefficient	Pa m <sup>3</sup> /mol	-	Calculated in S-Risk
Log K <sub>ow</sub> <sup>1</sup> K <sub>ow</sub>	g/g	4.49 (calculated value) <sup>(3)</sup> 30902,95	EpiSuite
Log K <sub>oc</sub> K <sub>oc</sub>	dm <sup>3</sup> /kg	2.57 (anion) 371.54	Higgins and Luthy (2006)
Log K <sub>oa</sub>	g/g	- <sup>(4)</sup>	optional in S-Risk
BCF	(mg/kg dm)/(mg/m <sup>3</sup> )	see table below	
Dpe	m <sup>2</sup> /d	1.10 <sup>-7</sup> (standard value)	Based on Vonk (1985) and Lijzen <i>et al.</i> (2011)
Dpvc	m <sup>2</sup> /d	1.10 <sup>-10</sup> (Dpe/1000)	Cornelis <i>et al.</i> (2017)
Diffusion for organic substance in air (Da)	m <sup>2</sup> /d	-	Calculated in S-Risk
Diffusion for organic substance in water (Dw)	m <sup>2</sup> /d	-	Calculated in S-Risk
Kp	[cm/h]	9.5.10 <sup>-7</sup> (AFPO)	Washburn <i>et al.</i> (2005)
FA	-	1	Cornelis <i>et al.</i> (2017)
ABS dermal soil/dust	-	0	Xiao <i>et al.</i> (2015)
BTF beef	d/kg	0.071	Vestergren <i>et al.</i> (2013)
BTF sheepmeat	d/kg	0.387	Kowalczyk <i>et al.</i> 2012

<sup>1</sup> Entered in S-Risk but not used in further calculations

Parameter	Unit	Value	Source
BTF liver	d/kg	0.441	Vestergren <i>et al.</i> (2013)
BTF kidney	d/kg	1.201	(1) Kowalczyk <i>et al.</i> (2013)
BTF milk	d/kg	0.021	Vestergren <i>et al.</i> (2013)
BTF soil – egg	d/kg		
BTF food - egg	d/kg		
Carcinogenicity		Carc. 2	EG (2008)
Systemic effects threshold <sup>(5)</sup>			
TDI oral	mg/kg.d	$6.3 \cdot 10^{-7}$	EFSA 2020
TCA inhalatory	[mg/m <sup>3</sup> ]	$2,21 \cdot 10^{-6}$	calculated from TDI oral
TDI dermal	mg/kg.d	$6.3 \cdot 10^{-7}$	= TDI oral
smoothing - ages		adult	
Limit in air	mg/m <sup>3</sup>	-	
Limit in drinking water	mg/m <sup>3</sup>	0.1	EC (2018)
Crop standard	mg/kg fw		
Meat and edible offal standard			EU (2022) <sup>2</sup>
Beef	mg/kg fw	$3 \cdot 10^{-4}$	
Sheepmeat	mg/kg fw	$1 \cdot 10^{-3}$	
Liver	mg/kg fw	$6 \cdot 10^{-3}$	
Kidney	mg/kg fw	$6 \cdot 10^{-3}$	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	$1 \cdot 10^{-3}$	
Dietary background all age groups including children	mg/kg day	$7 \cdot 10^{-7}$ (1 - < 3 y)	EFSA (2020) Lower bound
		$8.1 \cdot 10^{-7}$ (3 - < 6 y)	
		$3.3 \cdot 10^{-7}$ (6 - < 10 y)	
		$3.3 \cdot 10^{-7}$ (10 - < 15 y)	
		$3.3 \cdot 10^{-7}$ (15 - < 21 y)	
		$3.3 \cdot 10^{-7}$ (21 - < 31 y)	
		$4.5 \cdot 10^{-7}$ (31 - < 61 y)	
		$4.9 \cdot 10^{-7}$ ( $\geq$ 61 y)	
Background potato	mg/kg fw	$3.74 \cdot 10^{-6}$	EFSA (2020) LB
Background root vegetables	mg/kg fw	$3.081 \cdot 10^{-6}$	EFSA (2020) LB
Background bulbous vegetables (onion, etc.)	mg/kg fw	$3.081 \cdot 10^{-6}$	EFSA (2020) LB
Background fruiting vegetables	mg/kg fw	$3.081 \cdot 10^{-6}$	EFSA (2020) LB

<sup>2</sup> [Publications Office \(europa.eu\)](https://publications.office.europa.eu)

Parameter	Unit	Value	Source
Background cabbage	mg/kg fw	$3.081 \cdot 10^{-6}$	EFSA (2020) LB
Background leafy vegetables	mg/kg fw	$3.081 \cdot 10^{-6}$	EFSA (2020) LB
Background legumes	mg/kg fw	$3.081 \cdot 10^{-6v}$	EFSA (2020) LB
Background beef	mg/kg fw	$2.842 \cdot 10^{-5}$	EFSA (2020) LB
Background offal	mg/kg fw	$8.665 \cdot 10^{-4}$	EFSA (2020) LB
Background milk	mg/kg fw	$7.67 \cdot 10^{-7}$	EFSA (2020) LB
Background butter	mg/kg fw	$3.773 \cdot 10^{-6}$	EFSA (2020) LB (Assimilated to <i>animal fat</i> )
Background eggs	mg/kg fw	$2.674 \cdot 10^{-4}$	EFSA (2020) LB
Background outdoor air	mg/m <sup>3</sup>	$1.4 \cdot 10^{-9}$	P50 value from Cornelis <i>et al.</i> (2009)
Background indoor air	mg/m <sup>3</sup>	$1.6 \cdot 10^{-9}$	Jahnke <i>et al.</i> (2007b) in Cornelis <i>et al.</i> (2009)
Background drinking water	mg/m <sup>3</sup>	0	Assimilated to zero since it is included in the intake estimation of EFSA (2020)

<sup>(1)</sup> in S-Risk 'no' is entered because the K<sub>d</sub> of dissociative substances is calculated from log K<sub>ow</sub>, which we want to avoid; for non-dissociative substances the K<sub>d</sub> is calculated from the K<sub>oc</sub>

<sup>(2)</sup> 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.

<sup>(3)</sup> Log K<sub>ow</sub> is mandatory in S-Risk, and is used to calculate K<sub>p</sub>, K<sub>oc</sub>, and transfer factors, unless an experimental value is entered. Experimental values are available for these three parameters.

<sup>(4)</sup> Log K<sub>oa</sub> is optional in S-Risk, which uses K<sub>oa</sub> in the calculation of transfer to plants; as experimental data are available for this purpose, a K<sub>oa</sub> value is not necessary.

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

## ANNEX B: PFOA EFSA 2020 SUBSTANCE SHEET

Parameter	Unit	Value	Source
Name		Perfluorooctanoic acid	
CAS number		335-67-1	
EC number		206-397-9	
Type		organic	
Dissociative		no <sup>(1)</sup>	
Acid constant (pKa)		2.8	Moody and Field (2000)
Molar mass	g/mol	414,07	
Water solubility	mg/l	9.5.10 <sup>3</sup> (25°C)	ECHA (2014)
Vapour pressure	Pa	1.7.10 <sup>-2</sup> (10°C)	Lijzen <i>et al.</i> (2018)
Henry coefficient	Pa m <sup>3</sup> /mol	-	Calculated in S-Risk
Log K <sub>ow</sub> <sup>3</sup> K <sub>ow</sub>	g/g	4.81 (calculated value) <sup>(2)</sup> 64565,42	EpiSuite
Log K <sub>oc</sub> K <sub>oc</sub>	dm <sup>3</sup> /kg	2.06 114.82	Higgins and Luthy (2006)
Log K <sub>oa</sub>	g/g	- <sup>(3)</sup>	optional in S-Risk
BCF	(mg/kg dm)/(mg/m <sup>3</sup> )	See table below	
Dpe	m <sup>2</sup> /d	1.10 <sup>-7</sup> (standard value)	Vonk (1985); Lijzen <i>et al.</i> (2018)
Dpvc	m <sup>2</sup> /d	1.10 <sup>-10</sup> (Dpe/1000)	Cornelis <i>et al.</i> (2017)
Diffusion for organic substance in air (Da)	m <sup>2</sup> /d	-	Calculated in S-Risk
Diffusion for organic substance in water (Dw)	m <sup>2</sup> /d	-	Calculated in S-Risk
Kp	[cm/h]	9.49.10 <sup>-7</sup>	Fasano <i>et al.</i> (2005)
FA	-	1	Cornelis <i>et al.</i> (2017)
ABS dermal soil/dust	-	0	Xiao <i>et al.</i> (2015)
BTF beef	d/kg	5,999.10 <sup>-3</sup>	Vestergren, 2013 and Kowalczyk <i>et al.</i> (2013)

<sup>3</sup> Entered in S-Risk but not used in further calculations

## References

Parameter	Unit	Value	Source
BTF sheepmeat	d/kg	$6,950.10^{-3}$	Vestergren, 2013 and Kowalczyk <i>et al.</i> (2013)
BTF liver	d/kg	$8,756.10^{-3}$	Vestergren, 2013 and Kowalczyk <i>et al.</i> (2013)
BTF kidney	d/kg	$1,945.10^{-3}$	Vestergren, 2013 and Kowalczyk <i>et al.</i> (2013)
BTF milk	d/kg	$5,686.10^{-3}$	Vestergren, 2013 and Kowalczyk <i>et al.</i> (2013)
BTF soil – egg	d/kg		
BTF food - egg	d/kg		
Carcinogenicity		Carc. 2	EC (2008)
Systemic effects threshold <sup>(4)</sup>			
TDI oral	mg/kg.d	$6.3.10^{-7}$	EFSA 2020
TCA inhalatory	mg/m <sup>3</sup>	$2,21.10^{-6}$	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) <sup>-1</sup>	0.07 <sup>(5)</sup>	US-EPA (2016d)
Unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	-	
Slope factor dermal	(mg/kg/d) <sup>-1</sup>	-	
Smoothing duration		lifelong	
Limit in air	mg/m <sup>3</sup>	-	
Limit in drinking water	mg/m <sup>3</sup>	0.1	EC (2018)
Crop standard	mg/kg fw		
Meat and edible offal standard			EU (2022) <sup>4</sup>
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	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	$3.10^{-4}$	
Dietary background all age groups including children	mg/kg day	$2.60.10^{-7}$ (1 - < 3 y)	EFSA (2020)
		$2.40.10^{-7}$ (3 - < 6 y)	Lower bound

<sup>4</sup> [Publications Office \(europa.eu\)](https://publications.office.europa.eu)

Parameter	Unit	Value	Source
		2.40.10 <sup>-7</sup> (6 - < 10 y)	
		1.30.10 <sup>-7</sup> (10 - < 15 y)	
		1.30.10 <sup>-7</sup> (15 - < 21 y)	
		1.60.10 <sup>-7</sup> (≥ 31 y)	
Background potato	mg/kg fw	4.19.10 <sup>-6</sup>	EFSA (2020) LB
Background root vegetables	mg/kg fw	6.365.10 <sup>-6</sup>	EFSA (2020) LB
Background bulbous vegetables (onion, etc.)	mg/kg fw	6.365.10 <sup>-6</sup>	EFSA (2020) LB
Background fruiting vegetables	mg/kg fw	6.365.10 <sup>-6</sup>	EFSA (2020) LB
Background cabbage	mg/kg fw	6.365.10 <sup>-6</sup>	EFSA (2020) LB
Background leafy vegetables	mg/kg fw	6.365.10 <sup>-6</sup>	EFSA (2020) LB
Background legumes	mg/kg fw	6.365.10 <sup>-6</sup>	EFSA (2020) LB
Background beef	mg/kg fw	2.826.10 <sup>-5</sup>	EFSA (2020) LB
Background offal	mg/kg fw	9.162.10 <sup>-5</sup>	EFSA (2020) LB
Background milk	mg/kg fw	0	EFSA (2020) LB
Background butter	mg/kg fw	2.339.10 <sup>-6</sup>	EFSA (2020) LB assimilated to <i>animal fat</i>
Background eggs	mg/kg fw	1.064.10 <sup>-4</sup>	EFSA (2020) LB
Background outdoor air	mg/m <sup>3</sup>	8.90.10 <sup>-9</sup>	Cornelis <i>et al.</i> (2009)
Background indoor air	mg/m <sup>3</sup>	8.90.10 <sup>-9</sup>	Assimilated to outdoor air
Background drinking water	mg/m <sup>3</sup>	0	Assimilated to 0 since it is included in the intake estimation of EFSA (2020)

<sup>(1)</sup> in S-Risk 'no' is entered because the K<sub>d</sub> of dissociative substances is calculated from log K<sub>ow</sub>, which we want to avoid; for non-dissociative substances the K<sub>d</sub> is calculated from the K<sub>oc</sub>

<sup>(2)</sup> Log K<sub>ow</sub> is mandatory in S-Risk, and is used to calculate K<sub>p</sub>, K<sub>oc</sub>, and transfer factors, unless an experimental value is entered. Experimental values are available for these three parameters.

<sup>(3)</sup> Log K<sub>oa</sub> is optional in S-Risk, which uses K<sub>oa</sub> in the calculation of transfer to plants; as experimental data are available for this purpose, a K<sub>oa</sub> value is not necessary.

## References

<sup>(4)</sup> Due to the ongoing discussions on the new proposed TDI of EFSA, scenarios with 3 different sets of toxicological reference values will be calculated. The three sets are in the table below.

<sup>(5)</sup> The slope factor corresponds with a dose of  $1.43 \cdot 10^{-4}$  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 ( $2 \cdot 10^{-5}$  mg/kg bw/d) based on non-cancer effects is protective for the cancer endpoint (US-EPA, 2016b).

### BCF values PFOA

Plant	BCF or BCF model
<b>potatoes</b>	
potatoes	<b>0.06</b>
<b>root and tuber vegetables</b>	
carrots	<b>0.39</b>
salsify	0.55
	(average value of known root and tuber vegetables)
other root vegetables (such as radish)	<b>0.70</b>
<b>bulbous vegetables</b>	
	0.55
	(= average known root and tuber vegetables)
bulbous vegetables (such as onion)	0.55
	(= average known root and tuber vegetables)
leek	0.55
	(= average known root and tuber vegetables)
<b>fruiting vegetables</b>	
tomato	<b>0.81</b>
cucumber	<b>0.82</b>
other fruiting vegetables (such as peppers)	0.81 (=tomato)
<b>Cabbages</b>	
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)
<b>leafy vegetables</b>	
Lettuce	<b>1.90</b>
lamb's lettuce	1.90 (=sla)
endive	1.06
	(= average of all known leafy vegetables)
spinach	<b>0.87</b>
chicory	1.06
	(= average of all known leafy vegetables)



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Plant	BCF or BCF model
celery	<b>0.42</b>
<b>legumes</b>	
beans	0.03 (= peas)
peas	<b>0.03</b>
<b>Grasses</b>	
Grass	<b>0.128</b>
<b>Cereals</b>	
Maize	<b>0.005</b>