water

MDPI

Supplementary Materials

Review on Per- and Poly-Fluoroalkyl Substances' (PFASs') Pollution Characteristics and Possible Sources in Surface Water and Precipitation of China

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Table S1. Compound list of PFASs in the text.

Compound Name	Abbreviation	CAS Number	Molecular Formula	Molecular Weight (g/mol)	pK_a	log K_{ow}[a]
Tri-fluoroacetic acid	TFA	76-05-01	$C_2HF_3O_2$	114.02	/	/
Per-fluorobutanoic acid	PFBA	375-22-4	$C_4HF_7O_2$	214.04	0.17 [b]	2.14
Per-fluoropentanoic acid	PFPeA	2706-90-3	$C_5HF_9O_2$	264.05	0.40 ± 0.10 [b]	2.81
Per-fluorohexanoic acid	PFHxA	307-24-4	$C_6HF_{11}O_2$	314.05	−0.16 [c]	3.48
Per-fluoro-octanoic acid	PFOA	335-67-1	$C_8HF_{15}O_2$	414.07	−0.5 to 4.2 [c]	4.81
Per-fluoroethanesulfonic acid	PFEtS	354-88-1	$C_2HF_5O_3S$	200.08	/	/
Per-fluoropropanesulfonic acid	PFPrS	423-41-6	$C_3HF_7O_3S$	250.09	−3.63 ± 0.50 [b]	/
Per-fluorobutanesulfonic acid	PFBS	375-73-5	$C_4HF_9O_3S$	300.10	−3.31 [c]	1.82
Per-fluorohexane sulfonate acid	PFHxS	355-46-4	$C_6HF_{13}O_3S$	399.11	−3.45 [c]	3.16
Per-fluoro-octanesulfonic acid	PFOS	1763-23-1	$C_8HF_{17}O_3S$	500.13	<1.0 [c]	4.49
6:2 Fluorotelomer unsaturatedcarboxylic acid	FHUEA	70887-88-6	$C_8H_2F_{12}O_2$	358.08	2.96 ± 0.33 [b]	4.3
6:2 Fluorotelomer sulfonic acid	6:2 FTSA	27619-97-2	$C_8H_5F_{13}O_3S$	428.17	1.31 ± 0.50 [b]	2.66
6:2 Fluorotelomer unsaturated carboxylic acid	6:2 FTUCA	70887-88-6	$C_8H_2F_{12}O_2$	358.08	2.96 ± 0.33 [b]	4.3
8:2 Fluorotelomer unsaturated carboxylic acid	8:2 FTUCA	70887-84-2	$C_{10}H_2F_{16}O_2$	458.1	/	5.64
6:2 Fluorotelomer phosphate diester	6:2 diPAP	57677-95-9	$C_{16}H_9F_{26}O_4P$	790.17	/	9.42
8:2 Fluorotelomer phosphate diester	8:2 diPAP	678-41-1	$C_{20}H_9F_{34}O_4P$	990.2	1.36 ± 0.50 [b]	12.1
Per-fluoro-octane sulfonamide	FOSA	754-91-6	$C_8H_2F_{17}NO_2S$	499.15	7.01 ± 0.60 [b]	5.8
6:2 Chlorinated polyfluorinated ether sulphonic acid	6:2 Cl-PFESA (F-53B)	73606-19-6	$C_8F_{16}ClO(SO_3K)$	570.68	<1 [d]	5.24
Ammonium 4,8-dioxa-3H-per-fluorononanoic acid	ADONA	958445-44-8	$C_7H_5F_{12}NO_4$	395.06	/	3.56
Hexa-fluoropropylene oxide dimer acid	HFPO-DA	13252-13-6	$C_6F_{11}O_3H$	330.05	−0.06 [d]	3.36

Note: a, reference [34]; b, Chemicalbook (https://www.chemicalbook.com/ProductIndex.aspx); c, reference [58]; d, reference [59].

Table S2. Published administrative guidelines for PFOA and PFOS in water.

State/Country	Concentration Limit (ng/L)		Source
	PFOA	PFOS	
USEPA	70	70	(USEPA, 2016)
Alabama	400	200	(USEPA, 2009)
IIllinois	2	14	(EPA, 2021)
West Virginia	400	200	(USEPA, 2009)
Alaska	70	70	(AK DEC, 2018)
Australia	560	70	(ADEH, 2017)
Canada	200	600	(CAN HC, 2018)
Denmark	100	100	(EPA, 2015)
Germany	300	300	(GMOH, 2006)
Netherlands	390	200	(EPA, 2020)
Sweden	90	90	(NFA, 2014)
United Kingdom	10	10	(UKDWI, 2021)