Accessory publication

Using COSMOtherm to predict physicochemical properties of poly- and perfluorinated alkyl substances (PFASs)

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Table A1. Experimental physicochemical data for different groups of PFASs

Abbreviation	log K_{AW}	log $K_{OW, dry}$	log K_{OA}	log P_L (Pa)	log S_W (mg L^{-1})	log K_{OC} (L kg^{-1})
Perfluorinated carboxylate acids (PFCAs)						
PFOA	–2.99[A], –2.4/–2.1[B]			0.62[C], 0.71[D]		1.31–2.35[E], 2.06[F]
PFNA				0.10[C]		2.39 ± 0.09[F]
PFDA				–0.64[C]		2.76 ± 0.11[F]
PFUnA				–0.98[C]		3.30 ± 0.11[F]
PFDoA				–2.29[C]		
Perfluorinated sulfonic acids (PFSAs)						
PFOS						2.57 ± 0.13[F], 2.5–3.1[G]
PFDS						3.53 ± 0.12[F]
Fluorotelomer alcohols (FTOHs)						
4:2 FTOH	–1.52[H]	3.30 ± 0.04[I]	4.57 ± 0.55[J]	2.33[K]	2.99[L]	0.93[L]
6:2 FTOH	–0.56[H]	4.54 ± 0.01[I]	4.84 ± 0.71[J]	1.26[K]	1.27[L]	2.43[L]
8:2 FTOH	0.58[H]	5.58 ± 0.06[I]	5.58 ± 0.60[J]	0.60[K]	–0.86[M]	3.84[M]
10:2 FTOH	1.60[H]	6.63[I]	5.71 ± 0.47[J]	–0.70[K]	–1.96[L]	6.20[L]
12:2 FTOH			6.20 ± 0.49[J]			
Perfluoroalkanes						
PFBF				5.43[N]		
PFHxF				4.47[N]		
Perfluorinated alkyl sulfonamides (FASAs)						
N-MeFOSA			6.3 ± 0.3[O]			
N-EtFOSA			6.4 ± 0.3[O]			
N-MeFOSE			6.6 ± 0.5[O], 7.7[P]	–3.40[P]		
N-EtFOSE			6.7 ± 0.2[O], 7.8[P]	–2.77[P]		

[A]Li et al.[1]

[B]For p*K*a = 2.8/p*K*a = 1.3, Kutsuna and Hori.[2]

[C]Subcooled liquid phase, Kaiser et al.[3]

[D]Soild phase, Kutsuna and Hori.[4]

[E]DuPont EMSE Report.[5]

[F]Higgins and Luthy.[6]

[G]Johnson et al.[7]

[H]Goss et al.[8]

[I]Carmosini and Lee.[9]

[J]Thuens et al.[10]

[K]Subcooled liquid phase, Krusic et al.[11]

[L]Liu and Lee.[12]

[M]Liu and Lee.[13]

[N]Boublik et al.[14]

[O]Dreyer et al.[15]

[P]Solid phase vapour pressure, measured at 23ºC, K_{OA} were measured at 20ºC, Shoeib et al.[16]

Equation for calculating weighting factors based on Boltzmann distribution

In COSMOtherm, the probability of conformation *i* to occur, w_i, can be calculated according to the following equation, where the symmetry factors f_i represent the number of different possibilities to build the same structure. TFE_i denotes the total free energy (J mol^{-1}) of conformer *i*, including the total quantum chemical energy of conformer *i* in the ideal conductor, the correction of the screening charge energy and chemical potential of conformer *i* in the mixture. $TFE_{\min}$ is the total free energy (J mol^{-1}) of the conformer with the lowest free energy. R stands for the ideal gas constant (J mol^{-1} K^{-1}), and *T* stands for the absolute temperature (K).

$$w_i = \frac{f_i \cdot \exp\left\{-\frac{TFE_i - TFE_{\min}}{\mathrm{R}T}\right\}}{\sum_j f_j \exp\left\{-\frac{TFE_j - TFE_{\min}}{\mathrm{R}T}\right\}}$$

Table A2. List of the target chemicals (including CAS number and structures)

Chemical groups	Structures
Perfluorinated fatty acids	
Perfluorinated carboxylate acids (PFCAs)	CF_3-$(CF_2)_x$-**COOH**, *x* = 3,4,5…
Perfluorinated sulfonic acids (PFSAs)	CF_3-$(CF_2)_x$-**S(OH)O_2**, *x* = 3,5,7…
Perfluoroalkyl sulfinic acids (PFSiAs)	CF_3-$(CF2)_x$-**S(OH)O**, *x* = 3,5,7…
Perfluorinated phosphonic acids (PFPAs)	CF_3-$(CF_2)_x$-**PO(OH)$_2$**, *x* = 3,5,7…
Perfluoroalkyl phosphinic acids (PFPiAs)	CF_3-$(CF_2)_x$-**PO(OH)**-$(CF_2)_y$-CF_3, *x*, y = 5,7
Precursors	
Fluorotelomer alcohols (FTOHs)	CF_3-$(CF_2)_x$-**CH_2CH_2OH**, *x* = 1,3,5…
Fluorotelomer olefins (FTOs)	CF_3-$(CF_2)_x$-**CH=CH_2**, *x*=3,5,7…
Fluorotelomer sulfonate (FTSs)	CF_3-$(CF_2)_x$-**CH_2CH_2S(OH)O_2**, *x* = 1,3,5…
Fluorotelomer iodides (FTIs)	CF_3-$(CF_2)_x$-**CH_2CH_2I**, *x*=3,5,7…
Perfluoroalkyl iodides (PFAIs)	CF_3-$(CF_2)_x$-**I**, *x*=3,4,5…
Perfluoroalkyl sulfonamides (FASAs)	CF_3-$(CF_2)_x$-**SO_2NH_2**, *x* = 3,4,5…
N-Methyl perfluoroalkane sulfonamides (MeFASAs)	CF_3-$(CF_2)_x$-**SO_2NH(CH_3)**, *x* = 3,4,5…
N-Ethyl perfluoroalkane sulfonamides (EtFASAs)	CF_3-$(CF_2)_x$-**SO_2NH(C_2H_5)**, *x* = 3,4,5…
Perfluoroalkyl sulfonamido ethanols (FASEs)	CF_3-$(CF_2)_x$-**SO_2NH-CH_2CH_2OH**, *x*=3,4,5…
N-Methyl perfluoroalkane sulfonamido ethanols (MeFASEs)	CF_3-$(CF_2)_x$-**SO_2N(CH_3)-CH_2CH_2OH**, *x*=3,4,5…
N-Ethyl perfluoroalkane sulfonamido ethanols (EtFASEs)	CF_3-$(CF_2)_x$-**SO_2N(C_2H_5)-CH_2CH_2OH**, *x*=3,4,5…
Fluorotelomer phosphate monoesters (monoPAPs)	CF_3-$(CF_2)_x$-**CH_2CH_2-O-P(O)(OH)$_2$**, *x*=3,5,7…
Fluorotelomer phosphate diesters (diPAPs)	CF_3-$(CF_2)_x$-**CH_2CH_2O-P(OH)-OCH_2CH_2-**$(CF_2)_y$-CF_3, *x*, y=3,5,7…
Intermediates	
Fluorotelomer carboxylic acids (FTCAs)	CF_3-$(CF_2)_x$-**CH_2COOH**, *x* = 1,3,5…
Fluorotelomer unsaturated carboxylic acids (FTUCAs)	CF_3-$(CF_2)_x$-**CF=CHCOOH**, *x* = 0,2,4…
Fluorotelomer aldehyde (FTALs)	CF_3-$(CF_2)_x$-**CH_2CHO**, *x* = 1,3,5…
Fluorotelomer unsaturated aldehydes (FTUALs)	CF_3-$(CF_2)_x$-**CF=CHCHO**, *x* = 2,4,6…
Perfluorinated aldehyde (PFALs)	CF_3-$(CF_2)_x$-**CHO**, *x* = 3,4,5…

Table A3. Group 1: perfluoroalkyl acids – i. Perfluorinated carboxylate acids (PFCAs)

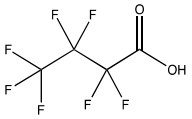
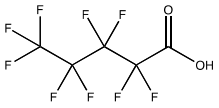
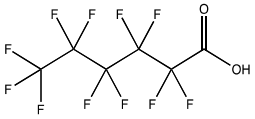
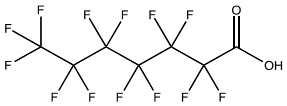
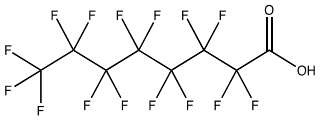
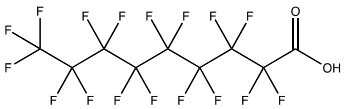
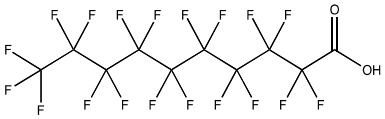
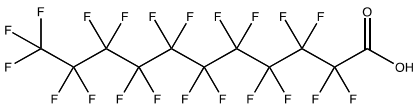
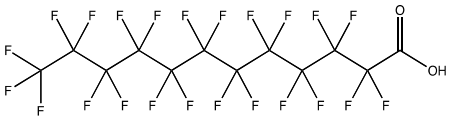
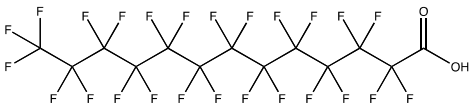
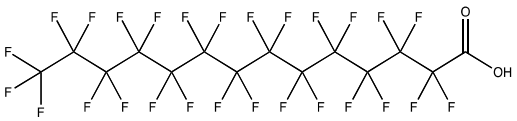
Abbreviation	Name	CAS number	Molecular structure
PFBA	perfluorobutanoic acid	375-22-4	
PFPeA	perfluoropentanoic acid	2706-90-3	
PFHxA	perfluorohexanoic acid	307-24-4	
PFHpA	perfluorohepanoic acid	375-85-9	
PFOA	perfluorooctanoic acid	335-67-1	
PFNA	perfluorononanoic acid	375-95-1	
PFDA	perfluorodecanoic acid	335-76-2	
PFUnDA	perfluoroundecanoic acid	2058-94-8	
PFDoDA	perfluorododecanoic acid	307-55-1	
PFTrDA	perfluorotridecanoic acid	72629-94-8	
PFTeDA	perfluorotetradecanoic acid	376-06-7	

Table A4. Group 1: perfluoroalkyl acids – ii. Perfluorinated sulfonic acids (PFSAs)

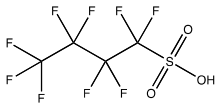
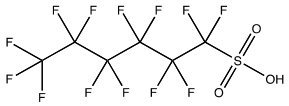
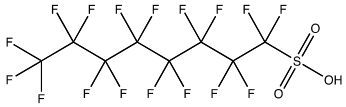
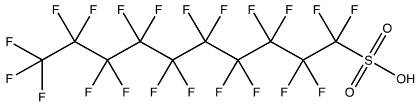
Abbreviation	Name	CAS number	Molecular structure
PFBS	perfluorobutanesulfonic acid	59933-66-3	
PFHxS	perfluorohexanesulfonic acid	355-46-4	
PFOS	perfluorooctanesulfonic acid	754-91-6	
PFDS	perfluorodecanesulfonic acid	335-77-3	

Table A5. Group 1: perfluoroalkyl acids – iii. Perfluoroalkyl sulfinic acids (PFSiAs)

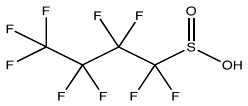
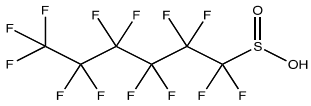
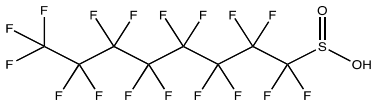
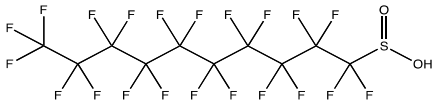
Abbreviation	Name	CAS number	Molecular structure
PFBSi	1,1,2,2,3,3,4,4,4-nonafluoro-1-butanesulfinic acid	34642-43-8	
PFHxSi	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfinic acid	115416-67-6	
PFOSi	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-1-octanesulfinic acid	647-29-0	
PFDSi	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10, 10,10-heneicosafluoro-1-decanesulfinic acid	558-98-5	

Table A6. Group 1: perfluoroalkyl acids – iv. Perfluoroalkyl phosphinic acids (PFPiAs)

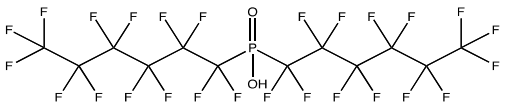
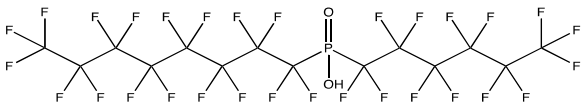
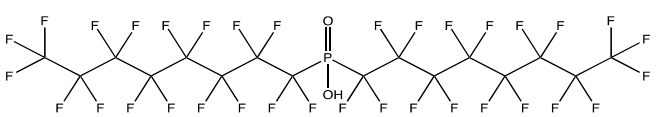
Abbreviation	Name	CAS number	Molecular structure
C6/C6 PFPiA	P,P-bis(1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexyl)-phosphinic acid	40143-77-9	
C6/C8 PFPiA	(heptadecafluorooctyl) (tridecafluorohexyl)-phosphinic acid	610800-34-5	
C8/C8 PFPiA	P,P-bis(1,1,2,2,3,3,4,4,5,5,6,6,7, 7,8, 8,8-heptadecafluorooctyl)-phosphinic acid	40143-79-1	

Table A7. Group 1: perfluoroalkyl acids – v. Perfluorinated phosphonic acids (PFPAs)

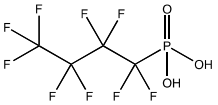
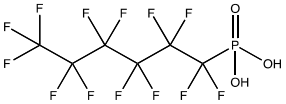
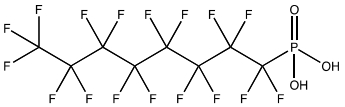
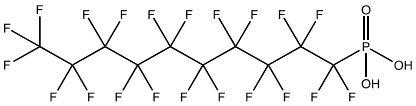
Abbreviation	Name	CAS number	Molecular structure
PFBPA	1,1,2,2,3,3,4,4,4-nonafluorobutyl phosphonic acid	52299-24-8	
PFHxPA	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexyl phosphonic acid	40143-76-8	
PFOPA	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctyl phosphonic acid	40143-78-0	
PFDPA	(perfluorodecyl)phosphonic acid	52299-26-0	

Table A8. Group 2: poly- and perfluorinated precursors – i. Fluorotelomer alcohols (FTOHs)

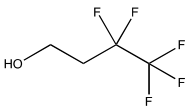
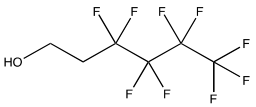
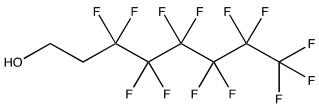
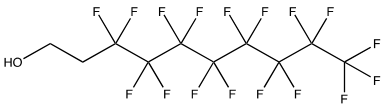
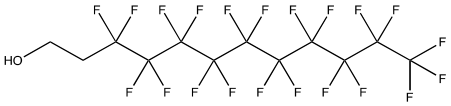
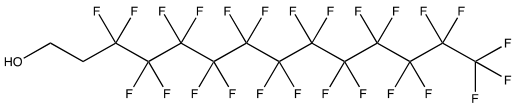
Abbreviation	Name	CAS number	Molecular structure
2:2 FTOH	2-(Perfluoroethyl)ethanol	54949-74-5	
4:2 FTOH	3,3,4,4,5,5,6,6,6-nonafluorohexan-1-ol	2043-47-2	
6:2 FTOH	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctan-1-ol	647-42-7	
8:2 FTOH	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecan-1-ol	678-39-7	
10:2 FTOH	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-henicosafluorododecan-1-ol	865-86-1	
12:2 FTOH	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecan-1-ol	39239-77-5	

Table A9. Group 2: poly- and perfluorinated precursors – ii. Fluorotelomer olefins (FTOs)

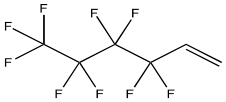
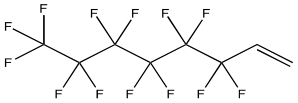
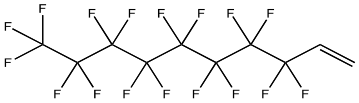
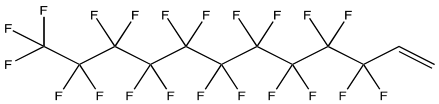
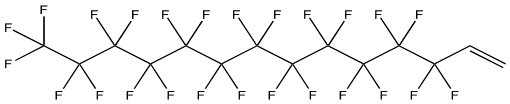
Abbreviation	Name	CAS number	Molecular structure
4:2 FTO	3,3,4,4,5,5,6,6,6-nonafluoro-1-hexene	19430-93-4	
6:2 FTO	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-octene	25291-17-2	
8:2 FTO	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decene	21652-58-4	
10:2 FTO	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluoro-1-dodecene	30389-25-4	
12:2 FTO	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluoro-1-tetradecene	67103-05-3	

Table A10. Group 2: poly- and perfluorinated precursors – iii. Perfluorinated alkyl sulfonamides (FASAs)

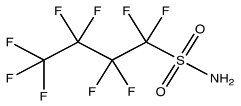
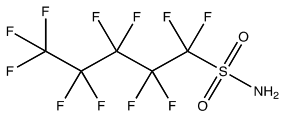
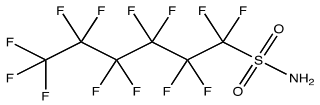
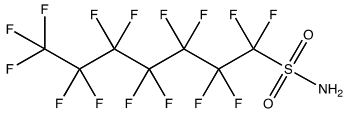
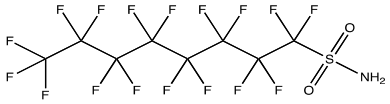
Abbreviation	Name	CAS number	Molecular structure
FBSA	1,1,2,2,3,3,4,4,4-nonafluoro-1-butanesulfonamide	30334-69-1	
FPeSA	1,1,2,2,3,3,4,4,5,5,5-undecafluoro-1-pentanesulfonamide	82765-76-2	
FHxSA	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonamide	41997-13-1	
FHpSA	1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-1-heptanesulfonamide	82765-77-3	
FOSA	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-1-octanesulfonamide	754-91-6	

Table A11. Group 2: poly- and perfluorinated precursors – iv. *N*-Methyl perfluoroalkane sulfonamides (MeFASAs)

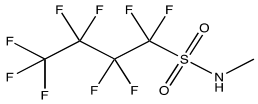
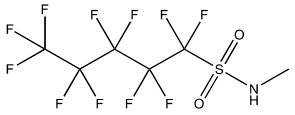
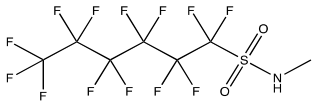
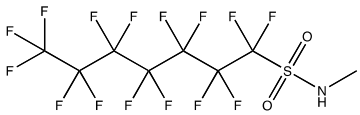
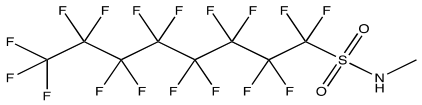
Abbreviation	Name	CAS number	Molecular structure
N-MeFBSA	1,1,2,2,3,3,4,4,4-nonafluoro-*N*-methyl-1-butanesulfonamide	68298-12-4	
N-MeFPeSA	1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-methyl-1-pentanesulfonamide	68298-13-5	
N-MeFHxSA	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-methyl-1-hexanesulfonamide	68259-15-4	
N-MeFHpSA	1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-methyl-1-heptanesulfonamide	68259-14-3	
N-MeFOSA	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-methyloctane-1-sulfonamide	31506-32-8	

Table A12. Group 2: poly- and perfluorinated precursors – v. *N*-Ethyl perfluoroalkane sulfonamides (EtFASAs)

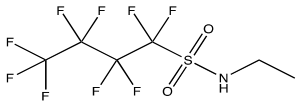
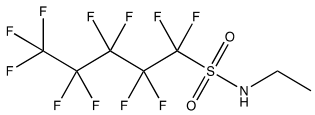
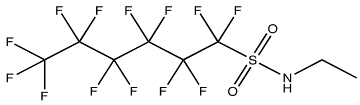
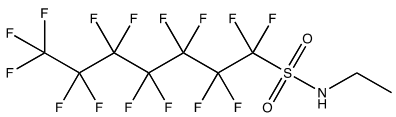
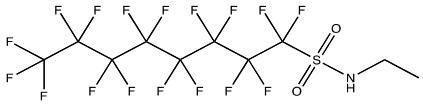
Abbreviation	Name	CAS number	Molecular structure
N-EtFBSA	*N*-ethyl-1,1,2,2,3,3,4,4,4-nonafluoro-1-butanesulfonamide	40630-67-9	
N-EtFPeSA	*N*-ethyl-1,1,2,2,3,3,4,4,5,5,5-undecafluoro-1-pentanesulfonamide	162682-16-8	
N-EtFHxSA	*N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonamide	87988-56-5	
N-EtFHpSA	*N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-1-heptanesulfonamide	68957-62-0	
N-EtFOSA	*N*-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane-1-sulfonamide	4151-50-2	

Table A13. Group 2: poly- and perfluorinated precursors – vi. Perfluoroalkyl sulfonamido ethanols (FASEs)

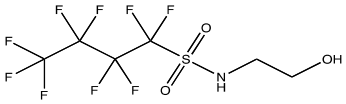
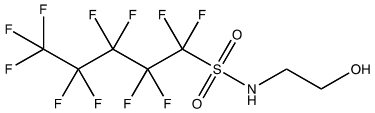
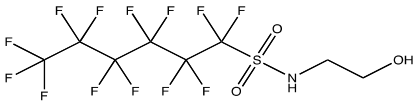
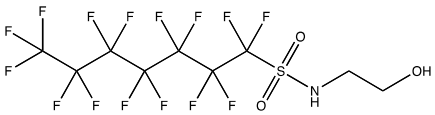
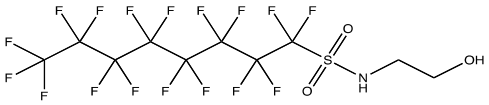
Abbreviation	Name	CAS number	Molecular structure
FBSE	1,1,2,2,3,3,4,4,4-nonafluoro-*N*-(2-hydroxyethyl)-1-butanesulfonamide	34454-99-4	
FPeSE	1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-(2-hydroxyethyl)pentane-1-sulfonamide	–	
FHxSE	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-(2-hydroxyethyl)-1-hexanesulfonamide	106443-63-4	
FHpSE	1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)-1-heptanesulfonamide	167398-54-1	
FOSE	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-1-octanesulfonamide	10116-92-4	

Table A14. Group 2: poly- and perfluorinated precursors – vii. *N*-Methyl perfluoroalkane sulfonamido ethanols (MeFASEs)

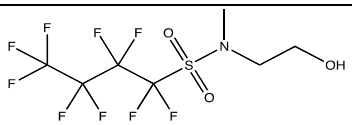
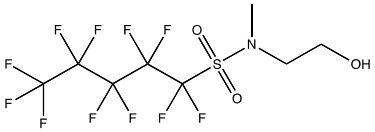
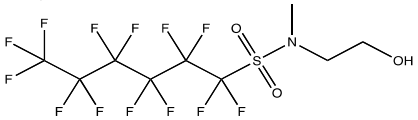
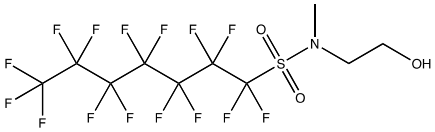
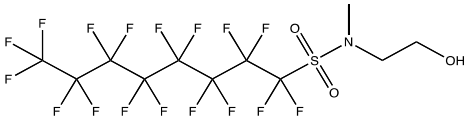
Abbreviation	Name	CAS number	Molecular structure
N-MeFBSE	1,1,2,2,3,3,4,4,4-nonafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-butanesulfonamide	34454-97-2	
N-MeFPeSE	1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-pentanesulfonamide	68555-74-8	
N-MeFHxSE	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-hexanesulfonamide	68555-75-9	
N-MeFHpSE	1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-heptanesulfonamide	68555-76-0	
N-MeFOSE	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyloctane-1-sulfonamide	24448-09-7	

Table A15. Group 2: poly- and perfluorinated precursors – viii. *N*-Ethyl perfluoroalkane sulfonamido ethanols (EtFASEs)

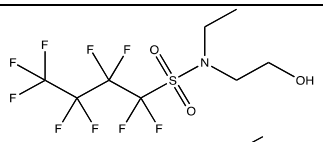
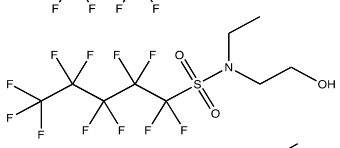
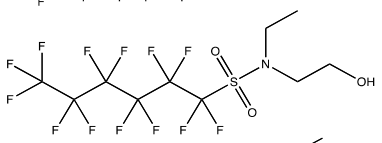
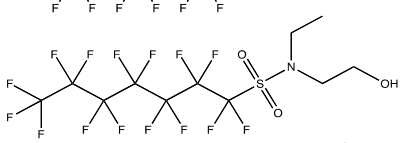
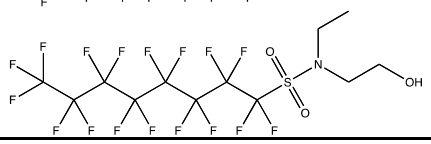
Abbreviation	Name	CAS number	Molecular structure
N-EtFBSE	1,1,2,2,3,3,4,4,4-nonafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-butanesulfonamide	34454-97-2	
N-EtFPeSE	1,1,2,2,3,3,4,4,5,5,5-undecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-pentanesulfonamide	68555-74-8	
N-EtFHxSE	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-hexanesulfonamide	68555-75-9	
N-EtFHpSE	1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyl-1-heptanesulfonamide	68555-76-0	
N-EtFOSE	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-*N*-(2-hydroxyethyl)-*N*-methyloctane-1-sulfonamide	24448-09-7	

Table A16. Group 2: poly- and perfluorinated precursors – ix. Fluorotelomer sulfonate (FTSs)

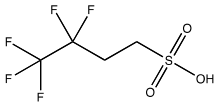
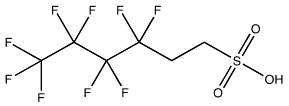
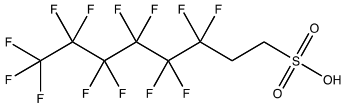
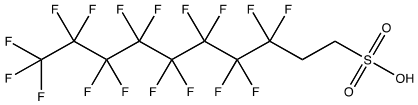
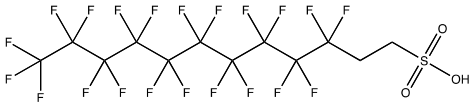
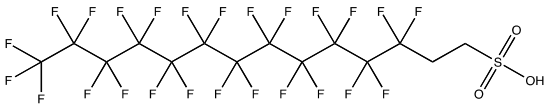
Abbreviation	Name	CAS number	Molecular structure
2:2 FTS	3,3,4,4,4-pentafluorobutane-1-sulfonic acid	149246-63-9	
4:2 FTS	3,3,4,4,5,5,6,6,6-nonafluorohexane-1-sulfonic acid	757124-72-4	
6:2 FTS	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctane-1-sulfonic acid	27619-97-2	
8:2 FTS	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecane-1-sulfonic acid	39108-34-4	
10:2 FTS	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-henicosafluorododecane-1-sulfonic acid	120226-60-0	
12:2 FTS	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecane-1-sulfonic acid	149246-64-0	

Table A17. Group 2: poly- and perfluorinated precursors – x. Fluorotelomer iodides (FTIs)

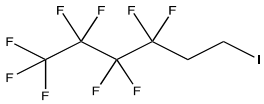
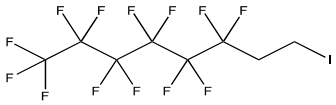
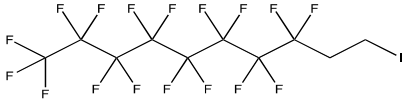
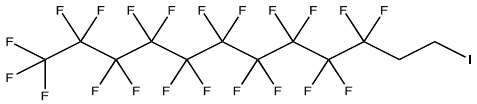
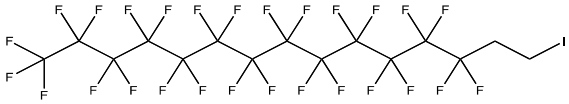
Abbreviation	Name	CAS number	Molecular structure
4:2 FTI	1,1,1,2,2,3,3,4,4-nonafluoro-6-iodo-hexane	2043-55-2	
6:2 FTI	1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodo-octane	2043-57-4	
8:2 FTI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-iodo-decane	2043-53-0	
10:2 FTI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafluoro-12-iodo-dodecane	2043-54-1	
12:2 FTI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13-heptacosafluoro-15-iodo-pentadecane	146983-96-2	

Table A18. Group 2: poly- and perfluorinated precursors – xi. Fluorotelomer phosphate monoesters (monoPAPs)

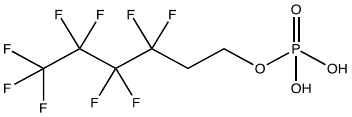
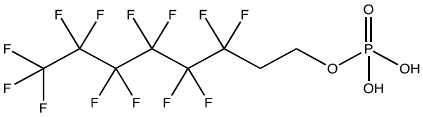
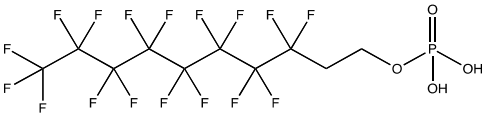
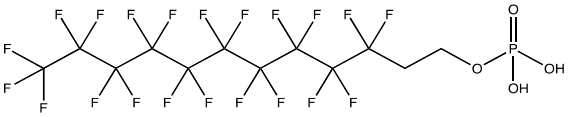
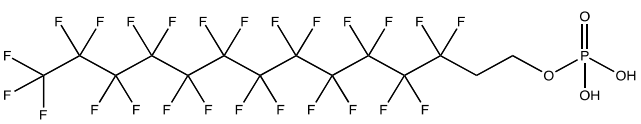
Abbreviation	Name	CAS number	Molecular structure
4:2 monoPAP	3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanol, 1-(dihydrogen phosphate)	150065-76-2	
6:2 monoPAP	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-octanol, 1-(dihydrogen phosphate)	57678-01-0	
8:2 monoPAP	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decanol, 1-(dihydrogen phosphate)	57678-03-2	
10:2 monoPAP	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluoro-1-dodecanol, 1-(dihydrogen phosphate)	57678-05-4	
12:2 monoPAP	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluoro-1-tetradecanol, 1-(dihydrogen phosphate)	57678-07-6	

Table A19. Group 2: poly- and perfluorinated precursors – xii. Perfluoroalkyl iodides (PFAIs)

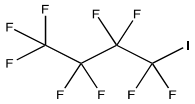
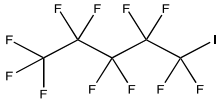
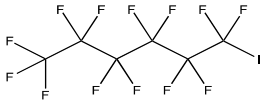
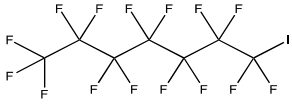
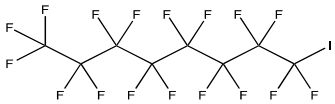
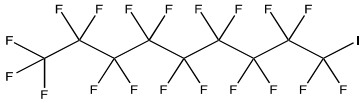
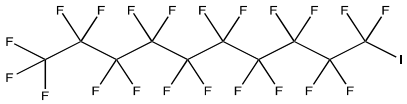
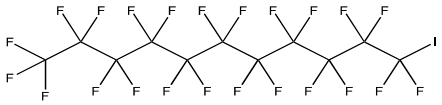
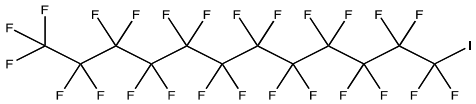
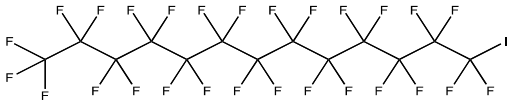
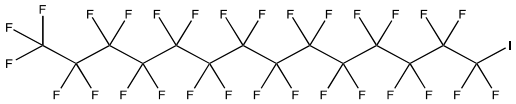
Abbreviation	Name	CAS number	Molecular structure
PFBI	1,1,1,2,2,3,3,4,4-nonafluoro-4-iodo-butane	423-39-2	
PFPeI	1,1,1,2,2,3,3,4,4,5,5-undecafluoro-5-iodo-pentane	638-79-9	
PFHxI	1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-iodo-hexane	355-43-1	
PFHpI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7-pentadecafluoro-7-iodo-heptane	335-58-0	
PFOI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-8-iodo-octane	507-63-1	
PFNI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-nonadecafluoro-9-iodo-nonane	558-97-4	
PFDI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-heneicosafluoro-10-iodo-decane	423-62-1	
PFUnDI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11-tricosafluoro-11-iodo-undecane	307-50-6	
PFDoDI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluoro-12-iodo-dodecane	307-60-8	
PFTrDI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13-heptacosafluoro-13-iodo-tridecane	376-04-5	
PFTeDI	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14-nonacosafluoro-14-iodo-tetradecane	307-63-1	

Table A20. Group 2: poly- and perfluorinated precursors – xiii. Fluorotelomer phosphate diesters (diPAPs)

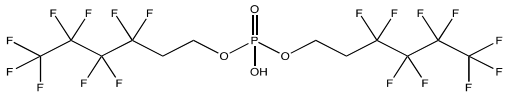
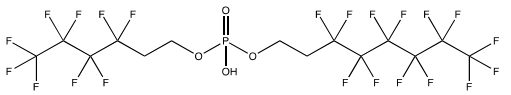
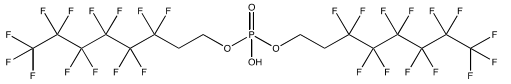
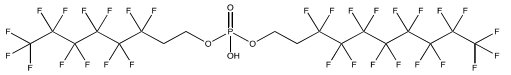
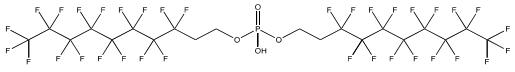
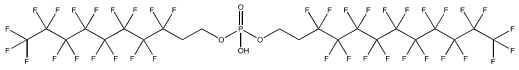
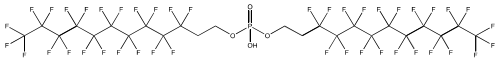
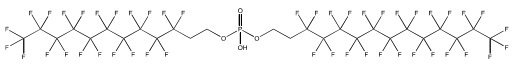
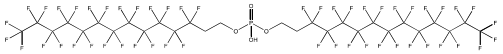
Abbreviation	Name	CAS number	Molecular structure
4:2 diPAP	bis(3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanol), hydrogen phosphate	135098-69-0	
4:2/6:2 diPAP	Phosphoric acid, mono(3,3,4,4,5,5,6,6,6-nonafluorohexyl) mono(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) ester	1158182-59-2	
6:2 diPAP	bis(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-1-octanol), hydrogen phosphate	57677-95-9	
6:2/8:2 diPAP	Phosphoric acid, mono(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-decyl) mono(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl) ester	943913-15-3	
8:2 diPAP	bis(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decanol), hydrogen phosphate	678-41-1	
8:2/10:2 diPAP	Phosphoric acid, mono(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl) mono(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) ester	1158182-60-5	
10:2 diPAP	bis(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10, 10,11,11,12,12,12-heneicosafluoro-1-dodecanol), hydrogen phosphate	1895-26-7	
10:2/12:2 diPAP	Phosphoric acid, mono(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-heneicosafluorododecyl) mono(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluoro-tetradecyl) ester	1158182-61-6	
12:2 diPAP	bis(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluoro-1-tetradecanol), hydrogen phosphate	57677-99-3	

Table A21. Group 3: poly- and perfluorinated intermediates – i. Fluorotelomer carboxylic acids (FTCAs)

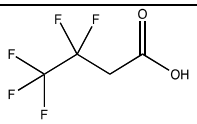
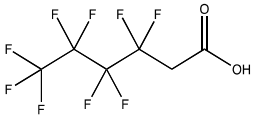
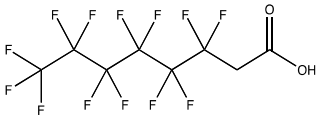
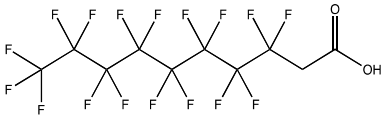
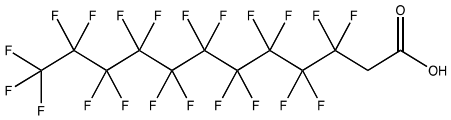
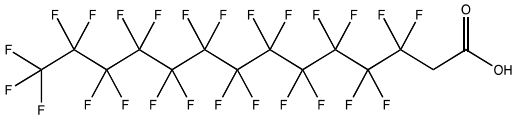
Abbreviation	Name	CAS number	Molecular structure
2:2 FTCA	3,3,4,4,4-pentafluorobutanoic acid	380-60-9	
4:2 FTCA	3,3,4,4,5,5,6,6,6-nonafluoro-hexanoic acid	70887-89-7	
6:2 FTCA	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanoic acid	53826-12-3	
8:2 FTCA	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecanoic acid	27854-31-5	
10:2 FTCA	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-henicosafluorododecanoic acid	53826-13-4	
12:2 FTCA	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecanoic acid	70887-93-3	

Table A22. Group 3: poly- and perfluorinated intermediates – ii. Fluorotelomer unsaturated carboxylic acids (FTUCAs)

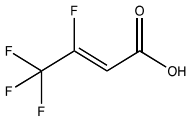
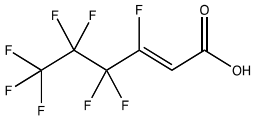
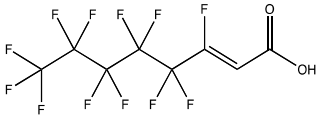
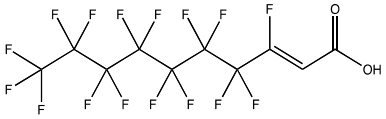
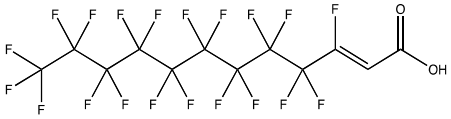
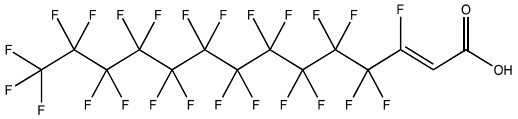
Abbreviation	Name	CAS number	Molecular structure
2:2 FTUCA	3,4,4,4-tetrafluorobut-2-enoic acid	70887-91-1	
4:2 FTUCA	3,4,4,5,5,6,6,6-octafluorohex-2-enoic acid	70887-90-0	
6:2 FTUCA	3,4,4,5,5,6,6,7,7,8,8,8-dodecafluorooct-2-enoic acid	70887-88-6	
8:2 FTUCA	3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-hexadecafluorodec-2-enoic acid	70887-84-2	
10:2 FTUCA	3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-icosafluorododec-2-enoic acid	70887-94-4	
12:2 FTUCA	3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-tetracosafluorotetradec-2-enoic acid	70887-95-5	

Table A23. Group 3: poly- and perfluorinated intermediates – iii. Perfluorinated aldehyde (PFALs)

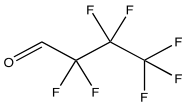
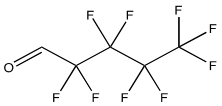
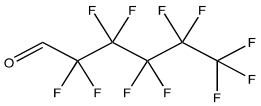
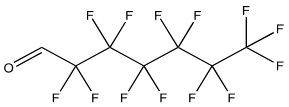
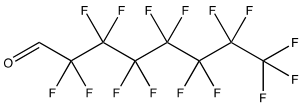
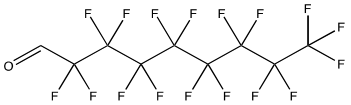
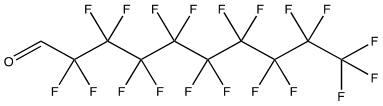
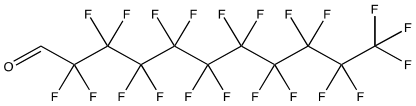
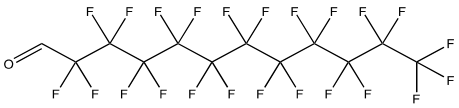
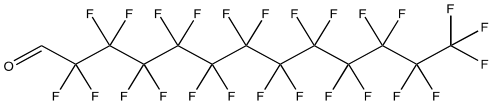
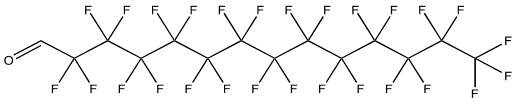
Abbreviation	Name	CAS number	Molecular structure
PFBAL	2,2,3,3,4,4,4-heptafluorobutanal	375-02-0	
PFPeAL	2,2,3,3,4,4,5,5,5-nonafluoropentanal	375-53-1	
PFHxAL	2,2,3,3,4,4,5,5,6,6,6-undecafluorohexanal	754-79-0	
PFHpAL	2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoroheptanal	63967-41-9	
PFOAL	2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanal	335-60-4	
PFNAL	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluorononanal	63967-40-8	
PFDAL	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-nonadecafluorodecanal	335-73-9	
PFUnDAL	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heneicosafluoroundecanal	63967-42-0	
PFDoDAL	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-tricosafluorododecanal	179799-68-9	
PFTrDAL	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,13-pentacosafluorotridecanal	–	
PFTeDAL	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-heptacosafluorotetradecanal	–	

Table A24. Group 3: poly- and perfluorinated intermediates – iv. Fluorotelomer aldehyde (FTALs)

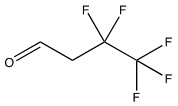
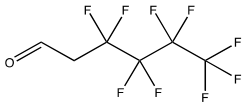
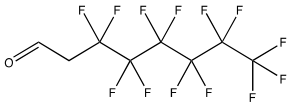
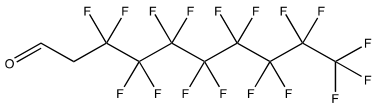
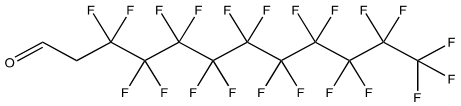
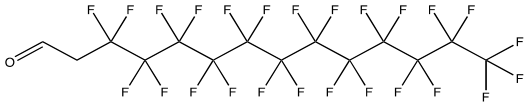
Abbreviation	Name	CAS number	Molecular structure
2:2 FTAL	3,3,4,4,4-pentafluorobutanal	239437-47-9	
4:2 FTAL	3,3,4,4,5,5,6,6,6-nonafluorohexanal	135984-67-7	
6:2 FTAL	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanal	56734-81-7	
8:2 FTAL	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecanal	135984-68-8	
10:2 FTAL	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-henicosafluorododecanal	864551-38-2	
12:2 FTAL	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecanal	–	

Table A25. Group 3: poly- and perfluorinated intermediates – v. Fluorotelomer unsaturated aldehydes (FTUALs)

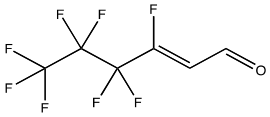
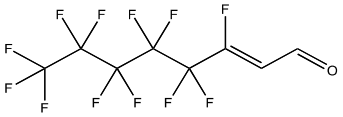
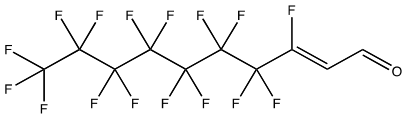
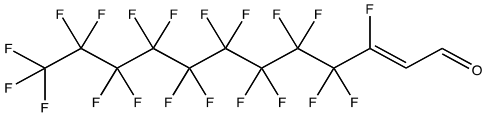
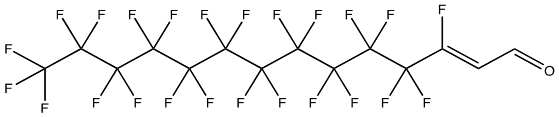
Abbreviation	Name	CAS number	Molecular structure
4:2 FTUAL	3,4,4,5,5,6,6,6-octafluoro-2-hexenal	864551-39-3	
6:2 FTUAL	3,4,4,5,5,6,6,7,7,8,8,8-dodecafluoro-2-octenal	69534-12-9	
8:2 FTUAL	3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-hexadecafluoro-2-decenal	58544-13-1	
10:2 FTUAL	3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-eicosafluoro-2-dodecenal	864551-40-6	
12:2 FTUAL	3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-tetracosafluorotetradec-2-enal	–	

Table A26. Group 4: Other poly- and perfluorinated chemicals – i. Perfluoroalkanes (PFFs)

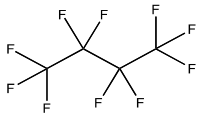
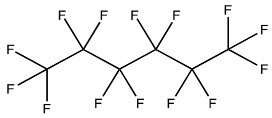
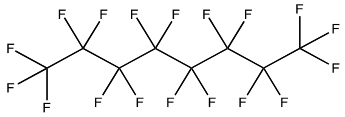
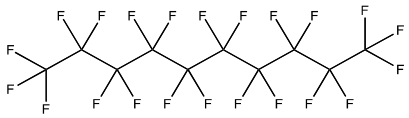
Abbreviation	Name	CAS number	Molecular structure
PFBF	1,1,1,2,2,3,3,4,4,4-decafluoro-butane	355-25-9	
PFHxF	1,1,1,2,2,3,3,4,4,5,5,6,6,6-tetradecafluoro-hexane	355-42-0	
PFOF	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-octadecafluoro-octane	307-34-6	
PFDF	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-docosafluoro-decane	307-45-9	

Table A27. Group 4: Other poly- and perfluorinated chemicals – ii. One substitute

DONA, new replacement of reported PFOA.[17]

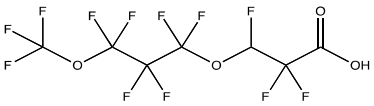
Abbreviation	Name	CAS number	Molecular structure
DONA	2,2,3-trifluoro-3-[1,1,2,2,3,3-hexafluoro-3-(trifluoromethoxy)propoxy]-propanoic acid	919005-14-4	

Table A28. Comparison of experimental data with estimates from COSMOtherm, EPISuite and SPARC

All the differences are calculated as 'experimental data – estimates'

Abbreviation	log K_{AW}	log $K_{OW, wet}$	log K_{OA}	log P_L (Pa)	log S_W (mg L^{-1})
Experimental data					
4:2 FTOH	–1.52	3.30	4.57	2.33	–2.43
6:2 FTOH	–0.56	4.54	4.84	1.26	–4.29
8:2 FTOH	0.58	5.58	5.58	0.60	–6.53
10:2 FTOH	1.60	6.63	5.71	–0.70	–7.71
Difference between the experimental data and COSMOtherm (CS 2.1 release 01.10)					
4:2 FTOH	0.18	0.70	0.21	0.03	–0.04
6:2 FTOH	0.55	0.69	–0.20	–0.09	–0.34
8:2 FTOH	0.94	0.60	0.13	0.04	–0.77
10:2 FTOH	1.12	0.41	–0.16	–0.44	0.08
Difference between the experimental data and COSMOtherm (CS 2.1 released before 2006)					
4:2 FTOH	–0.03	0.99	0.72	–0.02	–
6:2 FTOH	0.16	1.22	0.73	–0.30	–
8:2 FTOH	0.85	1.27	0.91	0.07	–
10:2 FTOH	0.94	1.24	0.87	–0.50	–
Difference between the experimental data and SPARC (ver. 4.5, September 2009)					
4:2 FTOH	0.85	0.69	–0.44	–0.07	–0.81
6:2 FTOH	0.43	0.10	–0.72	–0.70	–0.85
8:2 FTOH	–0.34	–1.04	–0.33	–1.02	–0.69
10:2 FTOH	–1.71	–2.51	–0.41	–2.04	0.65
Difference between the experimental data and SPARC (ver. February 2006)					
4:2 FTOH	1.12	1.08	–0.10	–0.26	–
6:2 FTOH	1.36	0.91	–0.52	–0.75	–
8:2 FTOH	1.39	0.27	–0.33	–0.96	–
10:2 FTOH	0.89	–0.66	–0.66	–1.86	–
Difference between the experimental data and EPISuite (ver. 4.0, January 2009)					
4:2 FTOH	–0.87	–0.36	0.26	–0.79	–1.30
6:2 FTOH	–1.35	–1.06	0.03	–0.86	0.82
8:2 FTOH	–1.65	–1.95	0.28	–0.51	–1.05
10:2 FTOH	–2.07	–2.83	–0.08	–0.82	–2.21
Difference between the experimental data and EPISuite (ver. February 2006)					
4:2 FTOH	–0.87	–0.36	0.26	–0.79	–
6:2 FTOH	–1.35	–1.06	0.03	–0.86	–
8:2 FTOH	–1.65	–1.95	0.28	–0.51	–
10:2 FTOH	–2.07	–2.83	–0.08	–0.82	–

Before a more detailed comparison is made, it is necessary to point out that we have chosen some new experimental data (for K_{OW} and K_{OA}) from some recent experimental studies: *i.* The K_{OW} values reported by Arp et al.[18] were estimated from experimental K_{OA} and K_{AW} values by using the thermodynamic triangle calculation, whereas the values used in this work are original experimental data with small variability[9]; ii. For K_{OA}, both studies have used similar experimental methods, however the values cited by Arp et al.[18] were only determined at three temperatures (0, 10, and 20ºC) [8]; whereas those used in this work were determined in a larger temperature range (eight measuring points within the range of 5–40ºC).[10]

Our modelled property data are generally in good agreement with data reported in Arp et al.[18] (Fig.2 in the main text, red dots), which were calculated with an earlier version of COSMOtherm. The differences could be due to different assumptions about which conformers were modelled, but because the two studies use different versions of the COSMOtherm software this cannot be confirmed. In particular, we used the newest version of COSMOtherm in which parameters were significantly improved for compounds containing F, Br, I, S and P.[19] Generally our prediction results show slightly better agreement (in the case of K_{OW} and K_{OA}) with measurement data than the results reported by Arp et al.[18]

Also we have compared the performance of COSMOtherm with EPISuite and SPARC (both data estimated with the newest version and the data published by Arp et al.[18]). It seems that the version update has not influenced the performance of EPISuite, whereas the estimated partition coefficients differed considerably between the two versions of SPARC. For the newest version of SPARC, some estimates have been improved and some have not. However, because there is no information given on the SPARC model website explaining the revisions that were made, it is not possible to explain the differences in estimates between mode versions. In general, both the SPARC and EPISuite methods are less accurate than COSMOtherm and the estimates vary up to several orders of magnitude.

Table A29. COSMOtherm results for FTOHs (including different conformers)

Exp., experimental data

Abbreviation	Conformer number	log K_{AW}	log $K_{OW,\ dry}$	log K_{OA}	log P_L (Pa)	log S_W (mol L^{-1})	log S_O (mol L^{-1})
4:2 FTOH	average	–1.70	2.66	4.36	2.31	–2.39	0.27
	#0-SC	–2.16	2.73	4.89	1.89	–2.34	0.38
	#1-EIC	–1.14	2.68	3.82	2.68	–2.58	0.10
	#2-SC	–2.88	2.47	5.34	1.39	–2.13	0.33
	Exp.	–1.52	3.30	4.57	2.33	–2.43	
6:2 FTOH	average	–1.11	3.93	5.04	1.34	–3.95	–0.02
	#0-SC	–1.47	3.98	5.46	1.02	–3.90	0.08
	#1-EIC	–0.56	3.96	4.52	1.70	–4.14	–0.18
	#2-SC	–2.11	3.78	5.88	0.55	–3.73	0.04
	Exp.	–0.56	4.54	4.84	1.26	–4.29	
8:2 FTOH	average	–0.36	5.08	5.45	0.56	–5.61	–0.53
	#0-EIC	0.10	5.12	5.02	0.84	–5.71	–0.67
	#1-SC	–1.59	4.90	6.50	–0.37	–5.20	–0.40
	#2-SC	–0.82	5.18	6.00	0.14	–5.48	–0.38
	Exp.	0.58	5.58	5.58	0.60	–6.53	
10:2 FTOH	average	0.48	6.35	5.87	–0.26	–7.79	–1.44
	#0-EIC	0.82	6.41	5.59	–0.08	–7.80	–1.47
	#1-SC	–0.78	6.26	7.04	–1.24	–7.35	–1.19
	#2-SC	–0.12	6.47	6.59	–0.77	–7.54	–1.17
	Exp.	1.60	6.63	5.71	–0.70	–7.71	

Table A30. Estimated physicochemical data for different groups of PFASs – i. Perfluoroalkyl acids

Values in the parentheses represent the available experimental data

Abbreviation	log K_{AW}	log $K_{OW, dry}$	log K_{OA}	log P_L (Pa)	log S_W (mol L^{-1})
Perfluorinated carboxylate acids (PFCAs)					
PFBA	–3.23	2.82	6.04	3.59	0.42
PFPeA	–2.90	3.43	6.33	3.13	–0.37
PFHxA	–2.58	4.06	6.63	2.66	–1.16
PFHpA	–2.25	4.67	6.92	2.20	–1.94
PFOA	–1.93 (–3.0)	5.30	7.23	1.73 (0.62)	–2.73
PFNA	–1.58	5.92	7.50	1.27 (0.10)	–3.55
PFDA	–1.27	6.50	7.77	0.82 (–0.64)	–4.31
PFUnDA	–0.92	7.15	8.08	0.34 (–0.98)	–5.13
PFDoDA	–0.58	7.77	8.36	–0.13 (–2.29)	–5.94
PFTrDA	–0.38	8.25	8.63	–0.57	–6.59
PFTeDA	0.03	8.90	8.87	–0.99	–7.42
Perfluorinated sulfonic acids (PFSAs)					
PFBS	–2.59	3.90	6.49	2.80	–1.00
PFHxS	–2.38	5.17	7.55	1.77	–2.24
PFOS	–1.65	6.43	8.07	0.83	–3.92
PFDS	–1.15	7.66	8.82	–0.15	–5.39
Perfluoroalkyl sulfinic acids (PFSiAs)					
PFBSi	–2.83	3.02	5.85	2.44	–1.12
PFHxSi	–2.18	4.23	6.41	1.56	–2.66
PFOSi	–1.53	5.48	7.01	0.63	–4.23
PFDSi	–0.78	6.77	7.55	–0.28	–5.90
Perfluorinated phosphonic acids (PFPAs)					
PFBPA	–8.76	2.19	10.95	–0.75	1.61
PFHxPA	–7.94	3.48	11.42	–1.44	0.11
PFOPA	–7.37	4.73	12.10	–2.29	–1.31
PFDPA	–6.95	5.98	12.93	–3.65	–3.09
Perfluoroalkyl phosphinic acids (PFPiAs)					
C6/C6 PFPiA	–1.51	8.08	9.59	–1.84	–6.72
C8/C8 PFPiA	–0.50	9.24	9.74	–2.28	–8.18
C6/C8 PFPiA	1.02	10.61	9.59	–3.03	–10.44

Table A31. Estimated physicochemical data for different groups of PFASs – ii. Precursors

Values in the parentheses represent the available experimental data

Abbreviation	log K_{AW}	log $K_{OW, dry}$	log K_{OA}	log P_L (Pa)	log S_W (mol L^{-1})	log S_O (mol L^{-1})
Fluorotelomer olefins (FTOs)						
4:2 FTO	1.76	3.86	2.10	4.23	–3.92	–0.07
6:2 FTO	2.39	5.09	2.70	3.23	–5.56	–0.47
8:2 FTO	3.05	6.34	3.29	2.23	–7.21	–0.88
10:2 FTO	3.71	7.57	3.86	1.26	–8.85	–1.28
12:2 FTO	4.37	8.80	4.43	0.28	–10.48	–1.68
Fluorotelomer sulfonate (FTSs)						
4:2 FTS	–5.80	3.21	9.02	–0.48	–1.07	–
6:2 FTS	–4.85	4.44	9.28	–0.96	–2.51	–
8:2 FTS	–4.52	5.66	10.18	–2.08	–3.96	–
10:2 FTS	–3.87	6.91	10.79	–2.95	–5.47	–
12:2 FTS	–2.91	7.94	10.85	–3.16	–6.65	–
Fluorotelomer iodides (FTIs)						
4:2 FTI	0.62	4.57	3.95	2.00	–5.01	–0.44
6:2 FTI	1.33	5.85	4.52	1.03	–6.70	–0.85
8:2 FTI	1.99	7.09	5.11	0.04	–8.34	–1.25
10:2 FTI	2.64	8.30	5.67	–0.92	–9.95	–1.65
12:2 FTI	3.58	10.21	6.63	–2.51	–12.49	–2.28
Perfluoroalkyl iodides (PFAIs)						
PFBI	2.20	4.32	2.15	3.55	–5.01	–0.70
PFPeI	2.51	4.93	2.43	3.05	–5.85	–0.92
PFHxI	2.83	5.55	2.72	2.54	–6.68	–1.14
PFHpI	3.15	6.16	3.01	2.04	–7.51	–1.35
PFOI	3.48	6.77	3.29	1.54	–8.33	–1.56
PFNI	3.81	7.38	3.57	1.05	–9.15	–1.77
PFDI	4.15	8.04	3.88	0.52	–10.03	–1.99
PFUnI	4.53	8.66	4.13	0.05	–10.87	–2.21
PFDoI	4.86	9.25	4.39	–0.41	–11.66	–2.41
PFTrI	5.03	9.90	4.86	–1.10	–12.53	–2.63
PFTeI	5.35	10.51	5.16	–1.60	–13.35	–2.84
Perfluoroalkyl sulfonamides (FASAs)						
FBSA	–3.51	3.16	6.67	1.02	–1.87	–
FPESA	–3.21	3.78	6.99	0.58	–2.60	–
FHXSA	–2.86	4.41	7.26	0.18	–3.36	–
FHpSA	–2.29	5.01	7.30	–0.17	–4.28	0.73
FOSA	–1.96	5.62	7.58	–0.61	–5.05	0.57
N-Methyl perfluoroalkane sulfonamides (MeFASAs)						
MeFBSA	–2.07	3.63	5.69	1.10	–3.23	0.40
MeFPeSA	–1.74	4.25	5.99	0.67	–3.98	0.27
MeFHxSA	–1.45	4.88	6.33	0.19	–4.76	0.12
MeFHpSA	–1.07	5.52	6.59	–0.24	–5.57	–0.06
MeFOSA	–0.58	6.07	6.64 (6.3)	–0.53	–6.35	–0.29
N-Ethyl perfluoroalkane sulfonamides (EtFASAs)						
EtFBSA	–1.89	4.14	6.03	0.76	–3.75	0.39
EtFPeSA	–1.33	4.93	6.26	0.32	–4.75	0.18
EtFHxSA	–1.08	5.46	6.54	–0.05	–5.37	0.09
EtFHpSA	–0.65	6.19	6.83	–0.58	–6.33	–0.14
EtFOSA	–0.36	6.71	7.07 (6.4)	–0.93	–6.97	–0.26
Perfluoroalkyl sulfonamido ethanols (FASEs)						

Abbreviation	log K_{AW}	log $K_{OW, dry}$	log K_{OA}	log P_L (Pa)	log S_W (mol L^{-1})	log S_O (mol L^{-1})
FBSE	–4.22	3.36	7.58	–0.57	–2.74	0.61
FPeSE	–4.04	3.89	7.93	–1.05	–3.41	0.48
FHxSE	–3.49	4.71	8.20	–1.40	–4.30	0.40
FHpSE	–3.35	5.25	8.59	–1.96	–5.01	0.24
FOSE	–2.99	5.78	8.76	–2.35	–5.76	0.02
N-Methyl perfluoroalkane sulfonamido ethanols (MeFASEs)						
MeFBSE	–3.34	3.76	7.11	–0.28	–3.34	0.42
MeFPeSE	–3.17	4.16	7.34	–0.76	–3.98	0.18
MeFHxSE	–2.92	4.91	7.83	–1.30	–4.78	0.13
MeFHpSE	–2.68	5.38	8.06	–1.72	–5.44	–0.06
MeFOSE	–2.35	6.00	8.35 (7.45)	–2.18 (–3.40)	–6.22	–0.22
N-Ethyl perfluoroalkane sulfonamido ethanols (EtFASEs)						
EtFBSE	–3.57	3.91	7.48	–0.75	–3.58	0.33
EtFPeSE	–3.22	4.72	7.95	–1.20	–4.37	0.35
EtFHxSE	–2.96	5.16	8.12	–1.61	–5.04	0.11
EtFHpSE	–2.50	5.93	8.43	–1.96	–5.85	0.08
EtFOSE	–2.08	6.52	8.59 (7.52)	–2.41 (–2.77)	–6.73	–0.21
Fluorotelomer phosphate monoesters (monoPAPs)						
4:2 monoPAP	–9.91	1.99	11.88	–4.06	–1.46	0.52
6:2 monoPAP	–9.33	3.39	12.72	–4.60	–2.24	–
8:2 monoPAP	–7.90	4.67	12.56	–4.85	–3.52	–
10:2 monoPAP	–7.17	5.92	13.09	–5.58	–4.80	–
12:2 monoPAP	–6.53	7.21	13.74	–6.53	–6.40	–
Fluorotelomer phosphate diesters (diPAPs)						
4:2 diPAP	–4.40	6.16	10.56	–4.13	–6.12	0.04
4:2/6:2 diPAP	–4.83	7.34	12.17	–6.08	–7.65	–0.31
6:2 diPAP	–4.16	8.41	12.57	–6.75	–8.98	–0.57
6:2/8:2 diPAP	–2.29	10.15	12.43	–6.91	–11.02	–0.87
8:2 diPAP	–2.55	10.93	13.48	–8.42	–12.26	–1.33
8:2/10:2 diPAP	–1.76	12.35	14.10	–9.16	–13.79	–1.45
10:2 diPAP	–2.44	12.88	15.31	–10.88	–14.84	–1.97
10:2/12:2 diPAP	–0.72	14.58	15.30	–11.22	–16.89	–2.31
12:2 diPAP	–1.01	15.15	16.16	–12.32	–17.71	–2.56

Table A32. Estimated physicochemical data for different groups of PFASs – iii. Intermediates

Abbreviation	log K_{AW}	log $K_{OW,\ dry}$	log K_{OA}	log P_L (Pa)	log S_W (mol L^{-1})	log S_O (mol L^{-1})
Fluorotelomer carboxylic acids (FTCAs)						
2:2 FTCA	–4.11	1.68	5.79	2.36	0.08	–
4:2 FTCA	–3.42	2.97	6.38	1.59	–1.39	–
6:2 FTCA	–2.80	4.14	6.94	0.76	–2.83	–
8:2 FTCA	–2.04	5.48	7.52	–0.11	–4.46	0.00
10:2 FTCA	–1.39	6.69	8.08	–0.96	–5.97	0.72
12:2 FTCA	–0.58	7.65	8.23	–1.39	–7.20	0.45
Fluorotelomer unsaturated carboxylic acids (FTUCAs)						
2:2 FTUCA	–3.49	1.68	5.17	2.92	0.01	–
4:2 FTUCA	–2.72	3.09	5.80	2.09	–1.58	–
6:2 FTUCA	–2.05	4.33	6.38	1.26	–3.09	–
8:2 FTUCA	–1.39	5.56	6.96	0.38	–4.62	–
10:2 FTUCA	–0.73	6.80	7.53	–0.52	–6.19	0.61
12:2 FTUCA	–0.04	8.07	8.11	–1.44	–7.80	0.27
Fluorotelomer aldehyde (FTALs)						
2:2 FTAL	–0.97	1.53	2.50	4.02	–1.40	0.13
4:2 FTAL	–0.35	2.76	3.11	3.15	–2.89	–0.14
6:2 FTAL	0.32	4.02	3.70	2.25	–4.46	–0.45
8:2 FTAL	0.99	5.24	4.25	1.36	–6.02	–0.79
10:2 FTAL	1.70	6.53	4.82	0.42	–7.67	–1.15
12:2 FTAL	2.33	7.74	5.41	–0.52	–9.24	–1.51
Fluorotelomer unsaturated aldehyde (FTUALs)						
4:2 FTUAL	0.19	2.86	2.68	3.63	–2.95	–0.09
6:2 FTUAL	0.84	4.10	3.26	2.71	–4.53	–0.43
8:2 FTUAL	1.50	5.34	3.84	1.77	–6.12	–0.79
10:2 FTUAL	1.96	6.54	4.58	0.68	–7.67	–1.13
12:2 FTUAL	2.60	7.78	5.18	–0.29	–9.29	–1.51
Perfluorinated aldehyde (PFALs)						
PFBAL	1.13	2.81	1.68	4.81	–2.71	0.09
PFPAL	1.50	3.43	1.93	4.35	–3.55	–0.12
PFHxAL	1.78	4.05	2.26	3.85	–4.33	–0.29
PFHpAL	2.11	4.60	2.49	3.40	–5.11	–0.51
PFOAL	2.43	5.28	2.85	2.86	–5.96	–0.68
PFNAL	2.75	5.89	3.13	2.39	–6.76	–0.88
PFDAL	3.06	6.52	3.45	1.89	–7.57	–1.06
PFUnAL	3.43	6.85	3.42	1.71	–8.12	–1.27
PFDoAL	3.77	7.78	4.02	0.89	–9.27	–1.49
PFTrAL	4.07	8.37	4.29	0.43	–10.04	–1.67
PFTeAL	4.33	8.61	4.28	0.26	–10.47	–1.86

Table A33. Estimated physicochemical data for different groups of PFAS – iv. Some other per- and polyfluorinated chemicals

Values in the parentheses represent the available experimental data. DONA, new replacement of reported PFOA[17]

Abbreviation	log K_{AW}	log $K_{OW,\ dry}$	log K_{OA}	log P_L (Pa)	log S_W (mol L^{-1})	log S_O (mol L^{-1})
Perfluoroalkanes (PFFs)						
PFBF	3.44	3.72	0.29	5.47 (5.43)	–4.37	–0.65
PFHxF	4.08	4.95	0.87	4.43 (4.47)	–6.04	–1.09
PFOF	4.75	6.21	1.46	3.40	–7.75	–1.54
PFDF	5.42	7.46	2.04	2.39	–9.43	–1.96
DONA	–2.94	4.85	7.80	1.37	–2.08	3.00

Comparison with available experimental data for the other PFASs

There are only relatively few experimental data for PFAS properties available in the literature. Our estimates of P_L agree well with the experimental data for perfluoroalkanes, but overestimate the values for several PFCAs, MeFOSE and EtFOSE. Moreover, COSMOtherm likely overestimates the K_{OA} values (for MeFOSA, EtFOSA, MeFOSE and EtFOSE) and the K_{AW} value for PFOA. Hence, a closer look at these substances is taken to further evaluate the overall performance of COSMOtherm.

For measured data of P_L of MeFOSE and EtFOSE, there are two experimental studies showing contradictory results. In one study, MeFOSE shows higher P_L than EtFOSE [20], while EtFOSE has a higher value in the other study.[16] A recent study observed that methylated sulfonamide and sulfonamide ethanols are more volatile than their ethylated counterparts [15], supporting the trends we observed. It is likely that the authors of the second study [16] have extrapolated the sub-cooled liquid vapour pressure (P_L) from the solid vapour pressure (P_S) incorrectly by using the same melting point and entropy of fusion for both compounds.[16] Although an exact phase correction cannot be made due to lack of information on the $\Delta_{fus}G$, it is likely that after correction our estimates will be within one log unit close to the empirical data.

For the P_L of PFOA, it is likely that in one experimental study [3] the vapour pressure was underestimated, since there is a contradiction with another value reported in the literature: the P_L is 4.2 Pa [3], whereas the other value, in this case for the solid phase, P_S, is 5.2 Pa.[4] It is possible that the extrapolation method (from high to low temperature) used in the first study [3] does not fit for PFOA (and the other PFCAs investigated). However, the vapour pressure measurements at different temperatures [3] allow us to calculate the enthalpy of vaporisation (ΔH_{VAP}) for PFOA (64.7 kJ mol^{-1}). If we combine this with the reported enthalpy of sublimation (ΔH_{SUB}), 88.9 kJ mol^{-1},[4] we obtain the enthalpy of fusion (ΔH_{FUS}) as 24.2 kJ mol^{-1} for PFOA. With this information we can correct the P_L estimated with COSMOtherm into P_S (20.9 Pa), which is approximately 4 times higher than the reported P_S of 5.2 Pa.[4] Therefore, we expect that COSMOtherm overestimates the vapour pressure of PFCAs, since it cannot consider the possible dimerisation level that can lower the vapour pressure. But the overestimation is still in a tolerable range.

For K_{OA}, COSMOtherm only slightly overestimates the values for perfluorinated sulfonamides (0.3 log units for MeFOSA and 0.6 log units for EtFOSA), whereas larger differences are observed between our estimates and the empirical data for MeFOSE and EtFOSE. Our estimates are 1.8 log units higher than in one study [15] and around one log unit higher than the value reported in another.[16] However, there is no clear evidence showing which experimental determination is more precise.

For the K_{AW} of PFOA, our estimate is around one log unit higher than the empirical value.[1] However, that empirical value was measured for the solute (including both the neutral species and its anionic form) in water having additional H_2SO_4 at 20ºC, whereas our estimate refers only to the neutral species in deionised water at 25ºC. Therefore, we have compared our estimated with another study that

excluded these confounding factors. Our estimate is close to the value corrected with pK_A = 1.3 (within 0.2 log units) and less close to the value corrected with pK_A =2.8 (within 0.5 log units).[2]

In combination with the results obtained for the FTOHs, it can be concluded that COSMOtherm estimates have some uncertainty, but at least for the cases where a comparison with measured data is possible, the uncertainty is at a tolerable level (within one order of magnitude close to the experimental data).

Table A34. Conformers generated by COSMOconf

Asterisks indicate that the conformation search was simplified as a result of too high computational requirement (if the complete conformation search is going to be done)

Abbreviations	Conformer number	Conformer type	Notice
Perfluorinated carboxylate acids (PFCAs)			
PFBA	2	SC, EIC	
PFPA	2	SC, EIC	
PFHxA	3	SC, EIC	
PFHpA	2	SC, EIC	
PFOA	2	SC, EIC	
PFNA	2	SC, EIC	
PFDA	2	SC, EIC	
PFUnA	1	SC	
PFDoA	1	SC	
PFTrA	1	SC	
PFTeA	1	SC	
Perfluorinated sulfonic acids (PFSAs)			
PFBS	3	SC	
PFHxS	2	SC	
PFOS	2	SC	
PFDS	1	SC	
Perfluoroalkyl sulfinic acids (PFSiAs)			
PFBSi	5	SC	
PFHxSi	4	SC	
PFOSi	3	SC	
PFDSi	4	SC	
Perfluorinated phosphonic acids (PFPhAs)			
PFBPhA	1	SC	
PFHxPhA	4	SC	
PFOPhA	1	SC	
PFDPhA	4	SC	
Perfluoroalkyl phosphinic acids (PFPiAs)			
C6/C6 PFPiA	2	SC	
C8/C8 PFPiA	1	SC	*
C6/C8 PFPiA	1	SC	*
Fluorotelomer olefins (FTOs)			
4:2 FTO	1	SC	
6:2 FTO	1	SC	
8:2 FTO	1	SC	
10:2 FTO	1	SC	
12:2 FTO	1	SC	
Perfluoroalkyl sulfonamides (FASAs)			
FBSA	2	SC	
FPESA	2	SC	
FHXSA	3	SC	
FHpSA	1	SC	
FOSA	2	SC	
N-Methyl perfluoroalkane sulfonamides (MeFASAs)			
N-MeFBSA	2	SC	
N-MeFPeSA	2	SC	
N-MeFHxSA	2	SC	
N-MeFHpSA	2	SC	
N-MeFOSA	1	SC	

Abbreviations	Conformer number	Conformer type	Notice
N-Ethyl perfluoroalkane sulfonamides (EtFASAs)			
N-EtFBSA	2	SC	
N-EtFPeSA	4	SC	
N-EtFHxSA	2	SC	
N-EtFHpSA	2	SC	
N-EtFOSA	1	SC	
Perfluoroalkyl sulfonamido ethanols (FASEs)			
FBSE	6	SC	
FPeSE	8	SC	
FHxSE	6	OxyEIC, SC	
FHpSE	7	SC	
FOSE	8	OxyEIC, SC	
N-Methyl perfluoroalkane sulfonamido ethanols (MeFASEs)			
N-MeFBSE	2	SC	
N-MeFPeSE	3	SC, OxyEIC	
N-MeFHxSE	3	SC	
N-MeFHpSE	2	SC	
N-MeFOSE	4	SC	
N-Ethyl perfluoroalkane sulfonamido ethanols (EtFASEs)			
N-EtFBSE	3	SC	
N-EtFPeSE	4	SC	
N-EtFHxSE	3	SC	
N-EtFHpSE	3	SC	
N-EtFOSE	4	SC, OxyEIC	
perfluoroalkyl iodides (PFAIs)			
PFBI	1	SC	
PFPeI	1	SC	
PFHxI	1	SC	
PFHpI	1	SC	
PFOI	1	SC	
PFNI	1	SC	
PFDI	1	SC	
PFUnI	1	SC	
PFDoI	1	SC	
PFTrI	1	SC	
PFTeI	1	SC	
Fluorotelomer iodides (FTIs)			
4:2 FTI	2	SC	
6:2 FTI	1	SC	
8:2 FTI	1	SC	
10:2 FTI	1	SC	
12:2 FTI	1	SC	
Fluorotelomer phosphate monoesters (monoPAPs)			
4:2 monoPAP	4	SC	
6:2 monoPAP	4	SC	
8:2 monoPAP	1	SC	*
10:2 monoPAP	1	SC	*
12:2 monoPAP	1	SC	*
Fluorotelomer phosphate diesters (diPAPs)			
4:2 diPAP	1	SC	*
4:2/6:2 diPAP	1	SC	*
6:2 diPAP	1	SC	*
6:2/8:2 diPAP	1	SC	*
8:2 diPAP	1	SC	*

Abbreviations	Conformer number	Conformer type	Notice
8:2/10:2 diPAP	1	SC	*
10:2 diPAP	1	SC	*
10:2/12:2 diPAP	1	SC	*
12:2 diPAP	1	SC	*
Fluorotelomer sulfonate (FTSs)			
4:2 FTS	3	SC	
6:2 FTS	4	SC	
8:2 FTS	1	SC	
10:2 FTS	1	SC	
12:2 FTS	1	SC	
Fluorotelomer carboxylic acids (FTCAs)			
2:2 FTCA	4	SC	
4:2 FTCA	3	SC	
6:2 FTCA	2	SC	
8:2 FTCA	3	SC	
10:2 FTCA	3	SC	
12:2 FTCA	1	SC	*
Fluorotelomer unsaturated carboxylic acids (FTUCAs)			
2:2 FTUCA	1	SC	
4:2 FTUCA	1	SC	
6:2 FTUCA	1	SC	
8:2 FTUCA	1	SC	
10:2 FTUCA	1	SC	
12:2 FTUCA	1	SC	
Fluorotelomer aldehyde (FTALs)			
2:2 FTAL	3	SC	
4:2 FTAL	2	SC	
6:2 FTAL	2	SC	
8:2 FTAL	2	SC	
10:2 FTAL	2	SC	
12:2 FTAL	1	SC	
Fluorotelomer unsaturated aldehydes (FTUALs)			
4:2 FTUAL	2	SC	
6:2 FTUAL	2	SC	
8:2 FTUAL	2	SC	
10:2 FTUAL	1	SC	
12:2 FTUAL	1	SC	
Perfluorinated aldehyde (PFALs)			
PFBAL	1	SC	
PFPAL	2	SC	
PFHxAL	1	SC	
PFHpAL	2	SC	
PFOAL	1	SC	
PFNAL	1	SC	
PFDAL	1	SC	
PFUnAL	1	SC	
PFDoAL	1	SC	
PFTrAL	1	SC	
PFTeAL	1	SC	

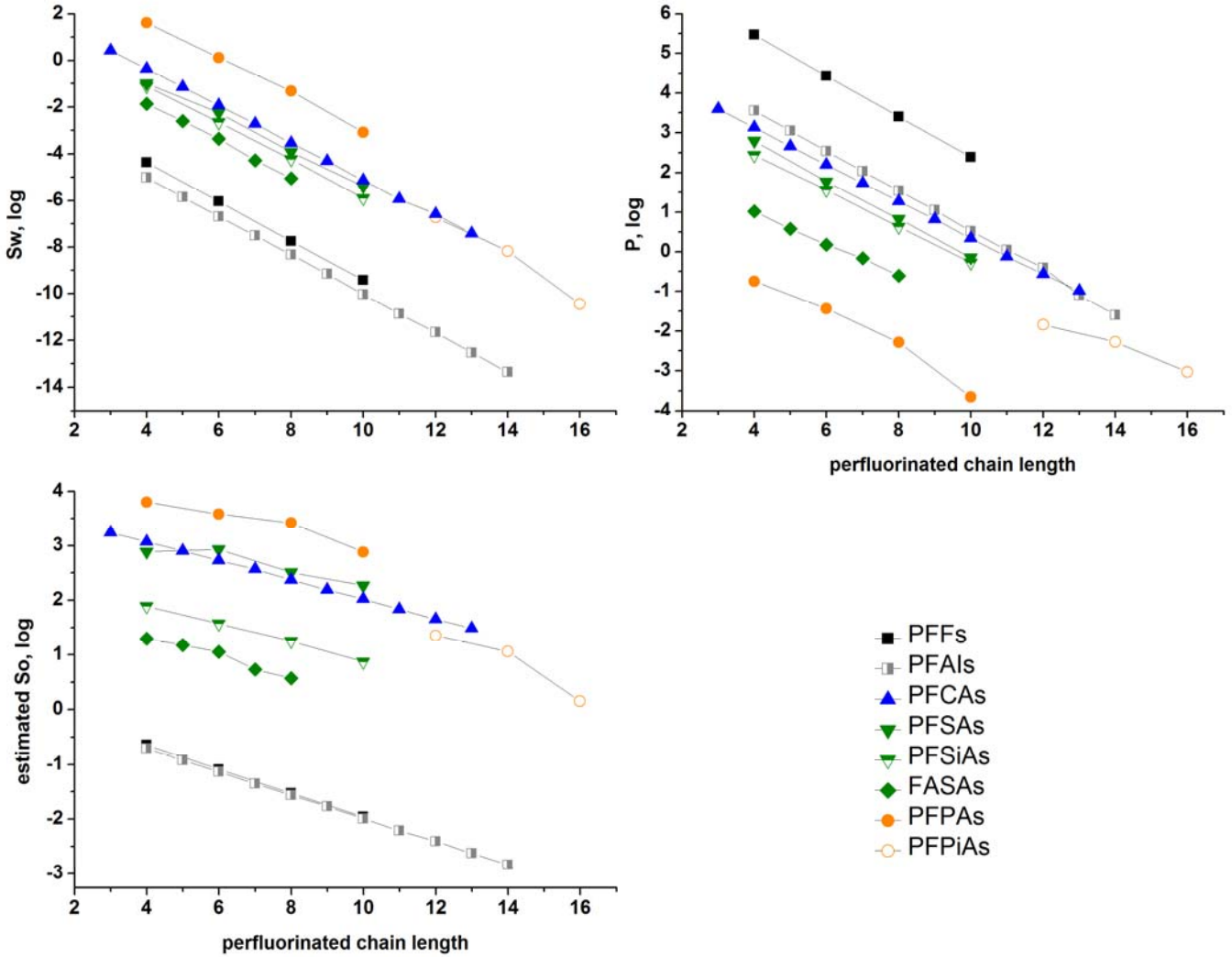


Fig A1. Influence of fluorinated chain length and functional group on P_L, S_W and S_O.

Table A35. Estimated physicochemical properties of branched isomers for C_4–C_7 PFCAs

Abbreviations are: m1, isomers with monomethyl branching pattern; m2, isomers with dimethyl branching patterns; e1, isomers with monoethyl branching pattern; m1e1, isomers with monomethyl-monoethyl branching patterns; a,b,c,d,e,f, stereoisomers. Molecular volume is in the unit of Å^3

Abbreviation	Name	log K_{AW}	log $K_{OW,\ dry}$	log K_{OA}	log P_L (Pa)	log S_W (mol L^{-1})	Molecular volume
c4m1	PFBA	–3.06	2.82	5.88	3.82	0.48	215.89
Linear	PFBA	–3.23	2.82	6.04	3.59	0.42	215.39
c5m1a	PFPeA	–2.98	3.24	6.21	3.23	–0.19	255.40
c5m1b	PFPeA	–2.75	3.42	6.17	3.44	–0.20	259.19
c5m2	PFPeA	–2.78	3.24	6.01	3.60	–0.02	251.38
Linear	PFPeA	–2.90	3.43	6.33	3.13	–0.37	258.32
c6e1	PFHxA	–2.47	4.01	6.48	3.00	–0.92	301.50
c6m1a	PFHxA	–2.77	3.80	6.57	2.75	–0.88	297.79
c6m1b	PFHxA	–2.64	3.81	6.46	2.83	–0.92	297.96
c6m1c	PFHxA	–2.36	4.04	6.40	2.99	–1.05	302.62
c6m2a	PFHxA	–2.11	3.54	5.65	3.02	–1.26	293.17
c6m2b	PFHxA	–2.44	3.77	6.21	3.09	–0.86	296.89
c6m2c	PFHxA	–2.42	3.73	6.15	3.29	–0.69	293.81
Linear	PFHxA	–2.58	4.06	6.63	2.66	–1.16	301.49
c7e1a	PFHpA	–2.53	4.23	6.76	2.40	–1.47	338.65
c7e1b	PFHpA	–2.04	4.59	6.63	2.57	–1.78	345.45
c7m1a	PFHpA	–2.42	4.43	6.85	2.32	–1.66	341.02
c7m1b	PFHpA	–2.54	4.31	6.85	2.34	–1.51	339.60
c7m1c	PFHpA	–2.33	4.40	6.73	2.35	–1.71	341.36
c7m1d	PFHpA	–2.00	4.64	6.64	2.50	–1.89	345.81
c7m1e1a	PFHpA	–2.30	4.28	6.58	2.84	–1.25	338.11
c7m1e1b	PFHpA	–2.36	4.20	6.57	2.98	–1.05	333.49
c7m2a	PFHpA	–2.89	3.61	6.50	2.09	–1.42	321.92
c7m2b	PFHpA	–2.10	4.40	6.49	2.65	–1.65	341.12
c7m2c	PFHpA	–2.29	4.22	6.51	2.66	–1.45	337.69
c7m2d	PFHpA	–2.56	4.04	6.60	2.61	–1.23	329.02
c7m2e	PFHpA	–2.47	4.02	6.49	2.74	–1.18	330.39
c7m2f	PFHpA	–2.11	4.34	6.45	2.85	–1.43	337.06
Linear	PFHpA	–2.25	4.67	6.92	2.20	–1.94	344.65

Table A36. Estimated pK_A values for some PFASs (including linear and branched isomers)

NA, not applicable, i.e. calculation cannot be conducted, as no reliable conformation of the PFHxPA anion can be found as a result of the limitation of the conformation search method

Abbreviation	Name	pK_A	Linear isomer	Branched isomer
c4m1	PFBA	0.69		X
PFBA	PFBA	0.85	X	
c5m1a	PFPeA	1.59		X
c5m1b	PFPeA	1.22		X
c5m2	PFPeA	1.29		X
PFPeA	PFPeA	0.81	X	
c6e1	PFHxA	1.45		X
c6m1a	PFHxA	2.36		X
c6m1b	PFHxA	2.07		X
c6m1c	PFHxA	1.11		X
c6m2a	PFHxA	0.05		X
c6m2b	PFHxA	1.63		X
c6m2c	PFHxA	1.65		X
PFHxA	PFHxA	0.84	X	
c7e1a	PFHpA	2.24		X
c7e1b	PFHpA	2.41		X
c7m1a	PFHpA	3.21		X
c7m1b	PFHpA	2.55		X
c7m1c	PFHpA	2.37		X
c7m1d	PFHpA	3.35		X
c7m1e1a	PFHpA	2.79		X
c7m1e1b	PFHpA	2.99		X
c7m2a	PFHpA	2.53		X
c7m2b	PFHpA	1.53		X
c7m2c	PFHpA	3.65		X
c7m2d	PFHpA	0.89		X
c7m2e	PFHpA	0.86		X
c7m2f	PFHpA	3.52		X
PFHpA	PFHpA	0.82	X	
P3MHpA[A]	PFOA	1.66		X
P4MHpA[A]	PFOA	1.59		X
P5MHpA[A]	PFOA	1.89		X
P6MHpA[A]	PFOA	0.89		X
PFOA	PFOA	0.90	X	
PFNA	PFNA	0.82	X	
PFBS	PFBS	–3.94	X	
PFHxS	PFHxS	–3.45	X	
PFOS	PFOS	–3.41	X	
PFDS	PFDS	–2.86	X	
PFBSi	PFBSi	1.69	X	
PFHxSi	PFHxSi	1.79	X	
PFOSi	PFOSi	1.81	X	
PFDSi	PFDSi	2.40	X	
PFBPA	PFBPA	1.06	X	
PFHxPA	PFHxPA	NA	X	
PFOPA	PFOPA	0.72	X	
PFDPA	PFDPA	0.60	X	

[A]These are stereoisomers of PFOA with a monomethyl branching pattern

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