CHAPTER 4. CHEMICAL AND PHYSICAL INFORMATION

4.1 CHEMICAL IDENTITY

Information regarding the chemical identity of perfluoroalkyls is located in Table 4-1. This information includes synonyms, chemical formulas and structures, and identification numbers. The perfluoroalkyls discussed in this profile exist as linear and branched isomers depending upon the method of production (see Chapter 5) and the reported values for the physical-chemical properties are typically reflective of the mixtures rather than a single specific isomer.

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of perfluoroalkyls is located in Table 4-2.

Perfluoroalkyls are very stable, owing to the strength of the carbon-fluorine bonds, the presence of the three electron pairs surrounding each fluorine atom, and the shielding of the carbon atoms by the fluorine atoms (3M 1999; Kissa 2001; Schultz et al. 2003). Perfluoroalkyl carboxylates and sulfonates are resistant to direct photolysis and reaction with acids, bases, oxidants, and reductants (3M 2000; EPA 2008a; OECD 2002, 2006a, 2007; Schultz et al. 2003).

APFO was shown to decompose starting at 196°C (Krusic and Roe 2004) and PFOA was shown to decompose rapidly in the presence of crushed borosilicate glass at 307°C (Krusic et al. 2005). 1-H perfluoroheptane and perfluoroheptene are noted degradation products.

Perfluoroalkyl carboxylates and sulfonates consist of a perfluorocarbon tail that is both hydrophobic and oleophobic and a charged end that is hydrophilic (3M 1999; de Vos et al. 2008; Kissa 2001; Schultz et al. 2003). This combination of hydrophobic and oleophobic characteristics makes these substances very useful as surfactants. The ability of these substances to repel oil, fat, and water has resulted in their use in surface protectants (Kissa 2001). Their ability to reduce the surface tension of aqueous systems to <20 mN/m has resulted in their use as wetting agents (Kissa 2001). Neutral or uncharged perfluoroalkyls or very long chain constituents are expected to form separate layers when mixed with hydrocarbons and water. Conversely, charged species, salts, and ionized species at relevant pH (i.e., PFOS, PFOA, PFHpA, PFNA) and short-chain species (i.e., PFBA, PFBS) have relatively good solubility in water and alcohol.

Table 4-1. Chemical Identity of Perfluoroalkyls

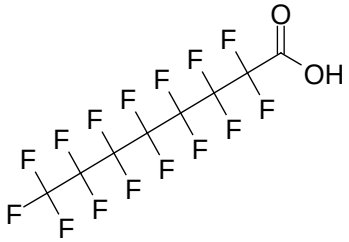
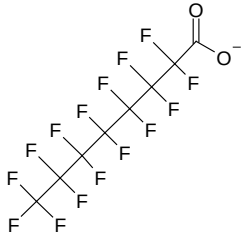
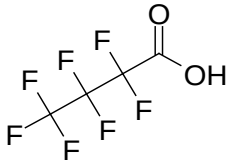
Characteristic	Information		
Chemical name	Perfluorooctanoic acid	Ammonium perfluorooctanoate	Perfluorobutanoic acid
Synonym(s)	PFOA; pentadecafluoro-1-octanoic acid; pentadecafluoro-n-octanoic acid; pentadecafluorooctanoic acid; perfluorocaprylic acid; perfluorooctanoic acid; perfluoroheptanecarboxylic acid; octanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8, 8-pentadecafluoro-	APFO; ammonium pentadecafluorooctanoate; octanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-ammonium salt (1:1)	PFBA; heptafluoro-1-butanoic acid; heptafluorobutanoic acid; heptafluorobutyric acid; perfluorobutyric acid; perfluoropropanecarboxylic acid; 2,2,3,3,4,4,4-heptafluorobutanoic acid
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_8HF_{15}O_2$	$C_8H_4F_{15}NO_2$	$C_4HF_7O_2$
Chemical structure			
CAS Registry Number	335-67-1	3825-26-1	375-22-4

Table 4-1. Chemical Identity of Perfluoroalkyls

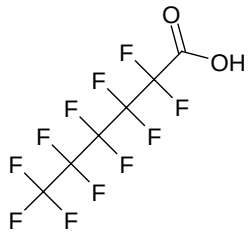
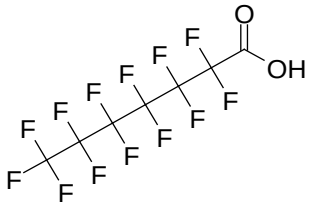
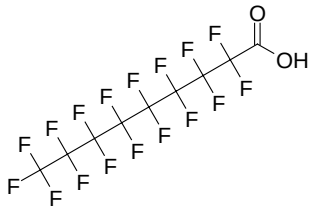
Characteristic	Information		
Chemical name	Perfluorohexanoic acid	Perfluoroheptanoic acid	Perfluorononanoic acid
Synonym(s)	PFHxA; undecafluoro-1-hexanoic acid; hexanoic acid, 2,2,3,3,4,4,5,5,6,6,6-undecafluoro-	PFHpA; perfluoro-n-heptanoic acid; tridecafluoro-1-heptanoic acid; heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-	PFNA; perfluoro-n-nonanoic acid; perfluorononan-1-oic acid; heptadecafluoro-nonanoic acid; nonanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluoro-
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_6HF_{11}O_2$	$C_7HF_{13}O_2$	$C_9HF_{17}O_2$
Chemical structure			
CAS Registry Number	307-24-4	375-85-9	375-95-1

Table 4-1. Chemical Identity of Perfluoroalkyls

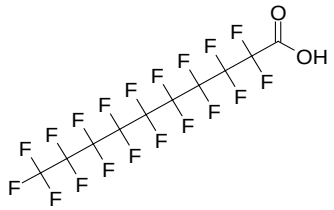
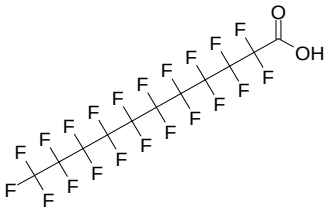
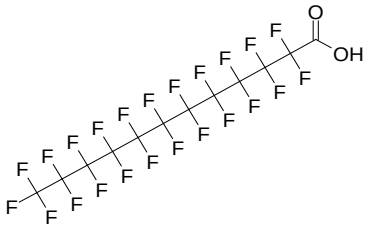
Characteristic	Information		
Chemical name	Perfluorodecanoic acid	Perfluoroundecanoic acid	Perfluorododecanoic acid
Synonym(s)	PFDA; PFDeA; Ndfda; nonadecafluoro-n-decanoic acid; nonadecafluorodecanoic acid; perfluoro-n-decanoic acid; decanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-nonadecafluoro-	PFUnA; perfluoro-n-undecanoic acid; henicosafluoroundecanoic acid; 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heneicosafluoroundecanoic acid	PFDoDA; tricosafluorododecanoic acid; dodecanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-tricosafluoro-
Registered trade name(s)	No data	No data	No data
Chemical formula	$C_{10}HF_{19}O_2$	$C_{11}HF_{21}O_2$	$C_{12}HF_{23}O_2$
Chemical structure			
CAS Registry Number	335-76-2	2058-94-8	307-55-1

Table 4-1. Chemical Identity of Perfluoroalkyls

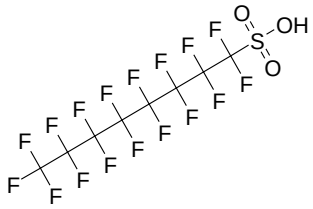
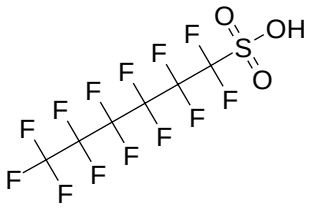
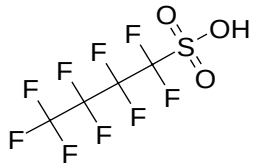
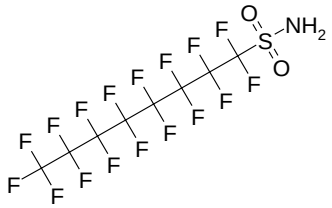
Characteristic	Information	
Chemical name	Perfluorooctane sulfonic acid	Perfluorohexane sulfonic acid
Synonym(s)	PFOS; 1-perfluorooctanesulfonic acid; heptadecafluoro-1-octanesulfonic acid; heptadecafluorooctan-1-sulphonic acid; perfluorooctane sulfonate; perfluorooctylsulfonic acid; 1-octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-	PFHxS; perfluorohexane-1-sulphonic acid; 1-hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-; 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexane-1-sulfonic
Registered trade name(s)	No data	No data
Chemical formula	$C_8HF_{17}O_3S$	$C_6HF_{13}O_3S$
Chemical structure		
CAS Registry Number	1763-23-1	355-46-4

Table 4-1. Chemical Identity of Perfluoroalkyls

Characteristic	Information	
Chemical name	Perfluorobutane sulfonic acid	Perfluorooctanesulfonamide
Synonym(s)	PFBS; 1-perfluorobutanesulfonic acid; nonafluoro-1-butanesulfonic acid; nonafluorobutanesulfonic acid; pentyl perfluorobutanoate; 1,1,2,2,3,3,4,4,4-nonafluoro-1-butanesulfonic acid; 1,1,2,2,3,3,4,4,4-nonafluoro-butane-1-sulphonic acid; 1-butanesulfonic acid, nonafluoro- (6Cl,7Cl,8Cl)	FOSA; perfluorooctylsulfonamide; perfluoro-octanesulfonic acid amide; heptadecafluorooctane-sulphonamide; 1-octanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-
Registered trade name(s)	No data	No data
Chemical formula	$C_4HF_9O_3S$	$C_8H_2F_{17}NO_2S$
Chemical structure		
CAS Registry Number	375-73-5	754-91-6

CAS = Chemical Abstracts Services

Sources: Calafat et al. 2007a, 2007b; CAS 2008; ChemIDplus 2008, 2017; RTECS 2008

Table 4-2. Physical and Chemical Properties of Perfluoroalkyls

Property	PFOA	APFO	PFBA	PFHxA
Molecular weight	414.069[a]	431.1[b]	214.039[a]	314.06[c]
Color	White to off-white[d]	No data	No data	Colorless[d]
Physical state	Solid[e]	Solid[b]	Liquid[a]	Liquid[d]
Melting point	54.3°C[a]	Decomposition starts above 105°C[b]	-17.5°C[a]	No data
Boiling point	188°C[a]	No data	121°C[a]	168°C at 742 mm Hg[f]
Density at 20°C	1.8 g/cm^3[g]	No data	1.651 g/cm^3[a]	1.789[f]
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	9.5x10^3 mg/L at 25°C[h] 2.29 x10^3 mg/L at 24°C[i] 3.3x10^3 mg/L at 25°C[j] 4.34x10^3 mg/L at 24.1°C[k]	>500 g/L[b]	2.14x10^5 mg/L at 25°C[l]	15,700 mg/L[m]
Organic solvents	No data	No data	Soluble in ethanol and toluene; insoluble in petroleum ether[a]	No data
Partition coefficients:				
Log K_{ow}	Not applicable[n]	No data	Not applicable[n]	Not applicable[n]
Log K_{oc}	1.69–2.36[o] 2.06[p]	K_{OC} 49–230[q]	2.17, average (n=7)[o]	2.06, average (n=7)[o]
pKa	-0.5[r] 0.5[s]	No data	0.08 (estimated)[t]	-0.16[m]
Vapor pressure	0.017 mm Hg at 20°C (extrapolated); 0.962 mm Hg at 59.25°C (measured)[u] 0.0316 mm Hg at 25°C[i]	0.0081 Pa at 20°C[b]	44 mm Hg at 56°C[h]	No data
Henry's law constant	0.362 Pa-m^3/mol[l]	No data	1.24Pa-m^3/mol[l]	No data
Autoignition temperature	Not applicable[v]	No data	Not applicable[v]	Not applicable[v]
Flashpoint	Not applicable[v]	No data	Not applicable[v]	Not applicable[v]
Flammability limits	Not applicable[u]	No data	Not applicable[u]	Not applicable[u]
Conversion factors	1 ppm=16.94 mg/m^3; 1 mg/m^3=0.059 ppm[w]	1 ppm=17.63 mg/m^3; 1 mg/m^3=0.057 ppm[w]	1 ppm=8.75 mg/m^3; 1 mg/m^3=0.11 ppm[w]	1 ppm=12.84 mg/m^3; 1 mg/m^3=0.078 ppm[w]
Explosive limits	Not applicable[v]	Not applicable[v]	Not applicable[v]	Not applicable[v]

Table 4-2. Physical and Chemical Properties of Perfluoroalkyls

Property	PFHpA	PFNA	PFDA	PFUnA
Molecular weight	364.06[u]	464.08[u]	514.084[t]	564.085[w]
Color	Beige[d]	No data	No data	No data
Physical state	Crystalline solid[d]	No data	No data	No data
Melting point	24–30°C[x]	No data	No data	97.9–100.3°C[x]
Boiling point	175°C at 742 mm Hg[h]	No data	219°C	No data
Density at 20°C	1.792 g/cm^3 [y]	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	4.37x10^5 mg/L at 25°C[l]	No data	No data	No data
Organic solvents	No data	No data	No data	No data
Partition coefficients:				
Log K_{ow}	Not applicable[n]	Not applicable[n]	Not applicable[n]	Not applicable[n]
Log K_{oc}	2.04, average (n=7)[o]	2.39[p]	2.79[p]	3.30[p]
pKa	-0.15 (estimated)[t] -2.29 (estimated)	-0.21 (estimated)[d]	-0.17 (estimated)[t]	-0.17 (estimated)[t]
Vapor pressure	4.6 mm Hg at 25°C[h] 0.133 at 25°C[d]	4.83x10^{-3} mm Hg at 20°C (extrapolated); 8.4 mm Hg at 99.63°C (measured)[t]	7.62x10^{-4} mm Hg at 20°C (extrapolated); 23.5 mm Hg at 129.56°C (measured)[aa]	3.44x10^{-4} mm Hg at 20°C (extrapolated); 4.62 mm Hg at 112.04°C (measured)[aa]
Henry's law constant at 25°C	0.573 Pa-m^3/mol[h]	No data	No data	No data
Autoignition temperature	Not applicable[v]	Not applicable[v]	Not applicable[v]	Not applicable[v]
Flashpoint	Not applicable[v]	Not applicable[v]	Not applicable[v]	Not applicable[v]
Flammability limits	Not applicable[v]	Not applicable[v]	Not applicable[v]	Not applicable[v]
Conversion factors	1 ppm=14.89 mg/m^3; 1 mg/m^3=0.067 ppm[w]	1 ppm=18.98 mg/m^3; 1 mg/m^3=0.053 ppm[w]	1 ppm=21.03 mg/m^3; 1 mg/m^3=0.048 ppm[w]	1 ppm=23.07 mg/m^3; 1 mg/m^3=0.043 ppm[w]
Explosive limits	Not applicable[v]	Not applicable[v]	Not applicable[v]	Not applicable[v]

Table 4-2. Physical and Chemical Properties of Perfluoroalkyls

Property	PFDoDA	PFOS	PFHxS
Molecular weight	614.1[c]	500.03[c]	400.12[c]
Color	No data	No data	No data
Physical state	No data	No data	No data
Melting point	No data	≥400°C (potassium salt)[z]	No data
Boiling point	No data	No data	No data
Density at 20°C	No data	No data	No data
Odor	No data	No data	No data
Odor threshold:			
Water	No data	No data	No data
Air	No data	No data	No data
Solubility:			
Water	No data	570 mg/L (potassium salt in pure water)[z]	No data
Organic solvents	No data	No data	No data
Partition coefficients:			
Log K_{ow}	Not applicable[j]	Not applicable[j]	Not applicable[j]
Log K_{oc}	No data	3.14, average (n=7)[o] 2.57[p]	2.28, average (n=7)[o]
pKa	-0.17 (estimated)[t]	0.14 (estimated)[t]	0.14 (estimated)[t]
Vapor pressure	5.11×10^{-60} mm Hg at 20°C (extrapolated)[z]	2.48×10^{-6} mm Hg at 20°C (potassium salt)[e]	No data
Henry's law constant at 25°C	No data	No data	No data
Autoignition temperature	Not applicable[v]	Not applicable[v]	Not applicable[v]
Flashpoint	Not applicable[v]	Not applicable[v]	Not applicable[v]
Flammability limits	Not applicable[v]	Not applicable[v]	Not applicable[v]
Conversion factors	1 ppm=25.12 mg/m^3; 1 mg/m^3=0.04 ppm[w]	1 ppm=20.45 mg/m^3; 1 mg/m^3=0.049 ppm[w]	1 ppm=16.36 mg/m^3; 1 mg/m^3=0.061 ppm[w]
Explosive limits	Not applicable[v]	Not applicable[v]	Not applicable[v]

Table 4-2. Physical and Chemical Properties of Perfluoroalkyls

Property	PFBS	FOSA
Molecular weight	300.1[c]	499.15[c]
Color	No data	No data
Physical state	No data	No data
Melting point	No data	No data
Boiling point	No data	No data
Density at 20°C	No data	No data
Odor	No data	No data
Odor threshold:		
Water	No data	No data
Air	No data	No data
Solubility:		
Water	No data	No data
Organic solvents	No data	No data
Partition coefficients:		
Log K_{ow}	Not applicable[n]	Not applicable[n]
Log K_{oc}	2.06 avg (n=7)[o]	No data
pKa	0.14 (estimated)[t]	6.24 (estimated)[t]
Vapor pressure	No data	No data
Henry's law constant	No data	No data
Autoignition temperature	Not applicable[v]	Not applicable[v]
Flashpoint	Not applicable[v]	Not applicable[v]
Flammability limits	Not applicable[v]	Not applicable[v]

Table 4-2. Physical and Chemical Properties of Perfluoroalkyls

Conversion factors	1 ppm=12.27 mg/m^3; 1 mg/m^3=0.081 ppm[u]	1 ppm=20.42 mg/m^3; 1 mg/m^3=0.049 ppm[w]
Explosive limits	Not applicable[u]	Not applicable[u]

[a]Lide 2005.
[b]EPA 2014.
[c]EPA 2008c.
[d]HSDB 2019.
[e]3M 2008c.
[f]Savu 1994a.
[g]Kroschwitz and Howe-Grant 1994.
[h]Kauck and Diesslin 1951.
[i]Bhhatarai and Gramatica 2011.
[j]Inoue et al. 2012.
[k]Rahman et al. 2014.
[l]Kwan 2001.
[m]Zhao et al. 2014.
[n]The log K_{ow} is not measurable since these substances are expected to form multiple layers in an octanol-water mixture (3M 1999, 2008c; EPA 2005a).
[o]McGuire et al. 2014.
[p]Higgins and Luthy 2006.
[q]Prevedouros et al. 2006.
[r]Goss 2008.
[s]Vierke et al. 2013.
[t]SPARC 2008.
[u]Kaiser et al. 2005.
[v]Perfluorocarboxylates and perfluorosulfonates are nonflammable (3M 1999, Kissa 2001, OECD 2007). However, they readily degrade via incineration (Krusic and Roe 2004; Krusic et al. 2005; Yamada et al. 2005).
[w]Calculated using molecular weight and the equation ppm=(X mg/m^3) x (24.45/molecular weight); mg/m^3=(X.ppm) x (molecular weight/24.45).
[x]ChemID Plus 2008.
[y]Kunleda and Shinoda 1976.
[z]Siegemund et al. 2015.
[aa]3M 2000.

APFO= ammonium perfluorooctanoate; FOSA = perfluorooctane sulfonamide; PFBA = perfluorobutanoic acid; PFBS = perfluorobutane sulfonic acid; PFDA = perfluorodecanoic acid; PFDoDA = perfluorododecanoic acid; PFHpA = perfluoroheptanoic acid; PFHxA = perfluorohexanoic acid; PFHxS = perfluorohexane sulfonic acid; PFNA = perfluorononanoic acid; PFOA = perfluorooctanoic acid; PFOS = perfluorooctane sulfonic acid; PFUnA = perfluoroundecanoic acid

The formation of an emulsified layer between the octanol and water interface makes the accurate measurement of properties such as log K_{ow} very difficult using conventional experimental techniques like the shake flask method or the slow stir technique (EPA 2005a, 3M 1999, 2008c). Xiang et al. (2018) used reverse-phase high-performance liquid chromatography (HPLC) to study the partitioning between the stationary column and mobile phase as a means of simulating the octanol-water partitioning process. As discussed in this study, acidic ionizable compounds are difficult to measure with this method since the pH of the mobile phase should be 2 log units lower than the pK_a of the chemical; however, extremely low pHs damage the stationary column. Therefore, a mobile phase over a range of pHs (1.09–5.00) was used to estimate the log D (sum of the ionized and unionized species in octanol/sum of the ionized and unionized species in water) over this pH range for 11 perfluoroalkylcarboxylic acids, including PFOA, and then the log D was converted to the neutral species log K_{ow}. The estimated log K_{ow} values of the perfluoroalkylcarboxylic acids (C4–C14) were in the range of 1.05 (PFBA) to 7.19 (perfluorotetra-decanoic acid).

Both the potential to form separate layers when mixed with hydrocarbons and water and the propensity for charged or ionized perfluoroalkyls to concentrate at interfaces make the measurement of the n-octanol water partition coefficient impractical (3M 1999; EPA 2005a).

The pKa range (Table 4-2) indicates that perfluoroalkyls will exist in anion form when in contact with water at environmental and physiologically relevant pHs. An estimated pKa of 6.24 indicates that FOSA will exist as both the anion and the neutral species (SPARC 2008). Perfluoroalkyl salts, such as APFO, will form the corresponding anions when dissolved in water. Prevedouros et al. (2006) reported a Krafft point of 22°C and critical micelle concentration of $3.7x10^3$ mg/L for the perfluorooctanoate anion (PFO). At temperatures above the Krafft point, the solubility of PFO is expected to increase abruptly due to the formation of micelles.

Vapor pressures at 25°C were extrapolated for PFOA, PFNA, PFDA, PFUnA, and PFDoDA using Antoine coefficients. Experimental vapor pressures were as follows: 0.962–724 mm Hg (59.25–190.80°C) for PFOA; 8.40–750 mm Hg (99.63–203.12°C) for PFNA; 23.5–750 mm Hg (129.56–218.88°C) for PFDA; 4.62–750 mm Hg (112.04–237.65°C) for PFUnA; and 6.42–750 mm Hg (127.58–247.36°C) for PFDoDA (Kaiser et al. 2005).