



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Perfluorooctane sulfonic acid(DD)
CAS #:	1763-23-1
Revised By:	RRD Toxicology Unit
Revision Date:	September 16, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	---	500.13	EPI	EXP
Physical State at ambient temp	---	Liquid	MDEQ	
Melting Point (°C)	---	NA	NA	NA
Boiling Point (°C)	---	258.00	EPI	EXP
Solubility (ug/L)	---	3.1	PC	EST
Vapor Pressure (mmHg at 25°C)	---	2.00E-03	PC	EST
HLC (atm-m³/mol at 25°C)	---	NA	NA	NA
Log Kow (log P; octanol-water)	---	6.28	PC	EST
Koc (organic carbon; L/Kg)	---	7.168E+04	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	---	3.02E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	---	3.52E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	---	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	---	NA	NA	NA
Lower Explosivity Level (LEL; unitless)	---	NA	NA	NA
Critical Temperature (K)		NA	NA	NA
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm ³)		NA	NA	NA
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	NA	EMSOFT	NA
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	NA	EMSOFT	NA
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	NA	EMSOFT	NA
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	NA	EMSOFT	NA

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	--	3.0E-5	USEPA, 2014	
RfD details		<p>Tier 3 Source: USEPA Office of Water: Basis: The RfD value from EPA Office of Water External Peer Review of EPA’s Draft Health Effects Documents for Perfluorooctanoic Acid (PFOA) and Perfluorooctane Sulfonate (PFOS) (2/2014) is selected because the assessment reviewed scientific information through 2013 and the final RfD protects for co-critical effects, developmental neurotoxicity and hepatotoxicity, and other developmental effects. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: Per MDEQ RRD (2011), RfD = 1.0E-5 mg/kg/day. Critical Study: Seacat et al (2002). Subchronic Toxicity Studies on Perfluorooctanesulfonate Potassium Salt in Cynomolgus Monkeys. <i>Toxicological Sciences</i>. 68: 249-264. (ecopy in tox assessment folder) Methods: animal: young-adult to adult male and female cynomolgus monkeys (n=6/sex/dose), duration: at least 26 weeks (183 days), doses: 0, 0.03 (n=4/sex), 0.15 or 0.75 mg/kg/day and treatment: oral Critical effect: hepatotoxicity and decreased triiodothyronine End point or Point of Departure (POD): NOAEL (human equivalent) = 0.003 mg/kg/day; NOAEL = 0.03 mg/kg/day Uncertainty Factors: UF = 300; 10 for intraspecies variability, 10 for subchronic to chronic extrapolation and 3 for the toxicodynamic component of the interspecies extrapolation Source and date: MDEQ RRD, 5/2011. See MDEQ RRD Toxicological Assessment</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>for additional information.</p> <p>EPA Office of Water: Per External Peer Review of EPA’s Draft Health Effects Documents for Perfluorooctanoic Acid (PFOA) and Perfluorooctane Sulfonate (PFOS) (2/2014), RfD= 0.00003 (3.0E-05) mg/kg/day. This value is selected based on the consistency of the response and with recognition of the use of developmental toxicity as the sensitive endpoint. This value is the outcome for the modeled rat serum for developmental neurotoxicity (Butenhoff et al., 2009) and supported by the slightly higher 0.00005 and 0.00006 mg/kg/day values for increases in liver weight and other developmental effects. Thus, co-occurring critical endpoints are protected by the chosen RfD.</p> <p>Critical Study: Butenhoff, J.L., D.J. Ehresman, S.-C. Chang, G.A. Parker, and D.G. Stump. 2009. Gestational and lactational exposure to potassium perfluorooctanesulfonate (K+PFOS) in rats: developmental neurotoxicity. <i>Reprod. Toxicol.</i> 27:319-330.</p> <p>Methods: Twenty five female Sprague-Dawley rats/group were administered 0, 0.1, 0.3 or 1.0 mg/kg/day potassium PFOS by gavage from gestation day (GD) 0 through postnatal day (PND) 20. An additional 10 mated females/group were used to collect additional blood and tissue samples. Offspring were monitored through PND 72 for growth, maturation, motor activity, learning and memory, acoustic startle reflex, and brain weight.</p> <p>Critical effects: developmental neurotoxicity (increased motor activity observed with decreased habituation).</p> <p>End point or Point of Departure (POD): NOAEL = 0.3 mg/kg-day PK-HED = 0.00088 mg/kg-day.</p> <p>Uncertainty Factors: UF = 30; 10 for intraspecies variability and 3 for toxicodynamic component of the interspecies extrapolation.</p> <p>Additional note: The most conservative potential RfD was derived from modeled serum for decreased pup body weight from a two-generation study (Luebker et al., 2005b). While this represents the most sensitive endpoint, it was described by the authors as a transient effect.</p>		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>EPA Office of Water: A PFOS provisional short-term value of 0.0002 mg/L is presented in the 2012 Drinking Water Standards and Health Advisories. The RfD used for deriving this value is not presented in the document.</p> <p>Minnesota DH: Per MDH, Toxicological Summary for Perfluorooctane Sulfonate, (5/4/2009), RfD = 8.00E-05 mg/kg/day: <u>Critical studies:</u> Thomford et al 2002 as cited by OECD 2002 and Seacat et al 2002. <u>Critical effect(s):</u> decreased HDL cholesterol, decreased total T3, increased TSH <u>Co-critical effect(s):</u> decreased body weight and body weight gain in offspring <u>Secondary effect(s):</u> changes in immune function, delayed development (e.g., body weight gain, eye opening), decreased adult body weight gain & loss of fat tissue, increased severity of liver effects (e.g., histological changes), disruption of estrus cycle, decreased sperm count & increased sperm deformities, decreased serum leptin levels, increased incidence of neoplasms (e.g., liver, thyroid, mammary gland), increased mortality (offspring and adults) <u>Point of Departure:</u> BMDL - 35 mg/L serum concentration <u>Human Equivalent Dose Adjustment:</u> 0.0025 mg/kg-d <u>Total uncertainty factor:</u> 30 (3 interspecies extrapolation and 10 intraspecies variability)</p> <p>Texas CEQ: RfD= 7.0E-04 mg/kg/day. This TCEQ derived value is based on...Details not readily available.</p> <p>European Food Safety Authority: TDI = 150 ng/kg/day (1.5E-4 mg/kg-day): This value is established by an EFSA panel (Perfluorooctane sulfonate (PFOS), perfluorooctanoic acid (PFOA) and their salts Scientific Opinion of the Panel on Contaminants in the Food Chain, 2008). <u>Key study:</u> Seacat, A.M., Thomford, P.J., Hansen, K.J., Olsen, G.W., Case, M.T. and Butenhoff, J.L. 2002. Sub chronic toxicity studies on perfluorooctanesulfonate potassium salt in</p>		



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>cynomolgus monkeys. Toxicol Sci. 68, 249-264. <u>Method:</u> Cynomolgus monkeys were administered orally with 0, 0.03, 0.15, or 0.75 mg PFOS/kg/day by oral intubation for 183 days. <u>Point of Departure:</u> lowest NOAEL = 0.03 mg/kg b.w. per day Overall uncertainty factor (UF): 200; 100 was used for inter and intra-species differences and an additional UF of 2 for uncertainties in connection to the relatively short duration of the key study and the internal dose kinetics.</p> <p>Other Tier 3: No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, Maine, Massachusetts, New Jersey, North Carolina and New York, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	Available data do not support the development of an oral SF at this time (9/27/11). See MDEQ RD Toxicological Assessment for additional information.	<p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ: Per DEQ-CCD, no value at this time. Based solely on the cancer model summary statistics, the incidence of hepatocellular carcinoma in female rats orally exposed to PFOS demonstrated the best model fit. However, the female hepatocellular carcinoma data set is represented by only a single observation of this tumor type that failed to demonstrate statistical significance from control values. Similarly, and despite statistically identified positive trends, the other evaluated data sets are represented by either extremely shallow cancer dose response curves or fail to effectively demonstrate any dose response relationship. Source: MDEQ-RRD, May 2011.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>EPA Office of Water: Per External Peer Review of EPA’s Draft Health Effects Documents for Perfluorooctanoic Acid (PFOA) and Perfluorooctane Sulfonate (PFOS) (2/2014), the weight of evidence for the carcinogenic potential to humans of these tumors was judged to be too limited to support a quantitative cancer assessment. In a chronic oral toxicity and carcinogenicity study of PFOS in rats, liver, thyroid and mammary fibroadenomas were identified (Thomford, 2002). The biological significance of the mammary fibroadenomas and thyroid tumors were questionable as a true dose-dependent response was not identified. Human epidemiology studies did not find a direct correlation between PFOS exposure and the incidence of carcinogenicity in worker-based populations. The induction of peroxisome proliferation has been suggested to be the mode of action (MOA) for the tumors observed with PFOS. While a number of short-term studies in rats and mice (Sohlenius et al., 1993; Ikeda et al., 1987; 3M Company, 2004) have shown that PFOS is capable of inducing peroxisome proliferation, longer-term studies in monkeys and rats have not (Seacat et al., 2002; 2003; Thomford, 2002).</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	--	NA	MDEQ, 2015	
RfC/ITSL details	No EPB-CCD entry for this chemical (9/27/11).	<p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD no value at this time.</p>		Complete
Inhalation Unit Risk Factor (IURF) ($(\mu\text{g}/\text{m}^3)^{-1}$)	NA	NA	MDEQ, 2015	
IURF details	No EPB-CCD entry for this chemical	<p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	(9/27/11).	<p>PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p>		
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
Developmental or Reproductive Effector? (Y/N)	No	Yes-oral , the RfD is based on a reproductive-developmental effect. Oral Exposure Pathways- Single Exposure	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	<p>The RfD is the outcome for the modeled rat serum for developmental neurotoxicity (Butenhoff et al., 2009) and supported by the slightly higher 0.00005 and 0.00006 mg/kg/day values for increases in liver weight and other developmental effects. Thus, co-occurring critical endpoints are protected by the chosen RfD.</p> <p>Critical Study: Butenhoff, J.L., D.J. Ehresman, S.-C. Chang, G.A. Parker, and D.G. Stump. 2009. Gestational and lactational exposure to potassium perfluorooctanesulfonate (K+PFOS) in rats: developmental neurotoxicity. <i>Reprod. Toxicol.</i> 27:319-330.</p> <p>Method(s): Twenty five female Sprague-Dawley rats/group were administered 0, 0.1, 0.3 or 1.0 mg/kg/day potassium PFOS by gavage from gestation day (GD) 0 through postnatal day (PND) 20. An additional 10 mated females/group were used to collect additional blood and tissue samples. Offspring were monitored through PND 72 for growth, maturation, motor activity, learning and memory, acoustic startle reflex, and brain weight.</p>		
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (µg/L)	--	NO	SDWA, 1976 and USEPA SMCL List	
SMCL details	--	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
Is there an Aesthetic Value? (Y/N)	No	Not evaluated.	NA	
Aesthetic value details	NA	NA		
Is there a Phytotoxicity Value? (Y/N)	No	Not evaluated.	NA	
Phytotoxicity details	NA	NA		
Others:				

(C) Chemical-specific Absorption Factors

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABS _{gi})	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS _{gi} details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (AE _d)	---	0.1	MDEQ, 2015	
AE _d details				
Ingestion Absorption Efficiency (AE _i)		0.5	MDEQ, 2015	
AE _i Details				
Relative Source Contribution for Water (RSC _w)		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC _s)		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC _A)		1.0	MDEQ, 2015	
Others				



(D) Rule 57 Water Quality Values and GSI Criteria

Current GSI value (µg/L)	NA
Updated GSI value (µg/L)	0.012 (X)
Rule 57 Drinking Water Value (µg/L)	0.011

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	0.011	3/2014
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	0.012	3/2014
Wildlife Value (WV)	NA	
Human Cancer Values for Drinking Water Source (HCV-drink)	NA	
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA	
Final Chronic Value (FCV)	140	8/2014
Aquatic maximum value (AMV)	780	8/2014
Final Acute Value (FAV)	1,600	8/2014

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)

(E) Target Detection Limits (TDL)

	Value	Source
Target Detection Limit – Soil ($\mu\text{g}/\text{kg}$)	NA	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	NA	MDEQ, 2015

CHEMICAL UPDATE WORKSHEET ABBREVIATIONS:

CAS # - Chemical Abstract Service Number.

Section (A) Chemical-Physical Properties**Reference Source(s):**

CRC	Chemical Rubber Company Handbook of Chemistry and Physics, 95th edition, 2014-2015
EMSOFT	USEPA Exposure Model for Soil-Organic Fate and Transport (EMSOFT) (EPA, 2002)
EPA2001	USEPA (2001) Fact Sheet, Correcting the Henry's Law Constant for Soil Temperature. Office of Solid Waste and Emergency Response, Washington, D.C.
EPA4	USEPA (2004) User's Guide for Evaluating Subsurface Vapor Intrusion into Buildings. February 22, 2004.
EPI	USEPA's Estimation Programs Interface SUITE 4.1, Copyright 2000-2012
HSDB	Hazardous Substances Data Bank
MDEQ	Michigan Department of Environmental Quality
NPG	National Institute for Occupational Safety and Health Pocket Guide to Chemical Hazards
PC	National Center for Biotechnology Information's PubChem database
PP	Syracuse Research Corporation's PhysProp database
SCDM	USEPA's Superfund Chemical Data Matrix
SSG	USEPA's Soil Screening Guidance: Technical Background Document, Second Edition, 1996
USEPA/EPA	United States environmental protection agency's Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment). July, 2004.

W9 USEPA's User Guide for Water9 Software, Version 2.0.0, 2001

Basis/Comments:

EST	estimated
EXP	experimental
EXT	extrapolated
NA	not available or not applicable
NR	not relevant

Section (B) Toxicity Values/Benchmarks**Sources/References:**

ATSDR	Agency for Toxic Substances and Disease Registry
CALEPA	California Environmental Protection Agency
CAL DTSC	California Department of Toxic Substances Control
CAL OEHHA	CAEPA Office of Environmental Health Hazard Assessment
CCD	MDEQ Chemical Criteria Database
ECHA	European Chemicals Agency (REACH)
OECD HPV	Organization for Economic Cooperation and Development HPV Database
HEAST	USEPA's Health Effects Assessment Summary Tables
IRIS	USEPA's Integrated Risk Information System
MADEP	Massachusetts Department of Environmental Protection
MDEQ/DEQ	Michigan Department of Environmental Quality
DEQ-CCD/AQD	MDEQ Air Quality Division
DEQ-CCD/RRD	MDEQ Remediation and Redevelopment Division
DEQ-CCD/WRD	MDEQ Water Resources Division
MNDOH	Minnesota Department of Health

NJDEP	New Jersey Department of Environmental Protection
NYDEC	New York State Department of Environmental Conservation
OPP/OPPT	USEPA's Office of Pesticide Programs
PPRTV	USEPA's Provisional Peer Reviewed Toxicity Values
RIVM	The Netherlands National Institute of Public Health and the Environment
TCEQ	Texas Commission on Environmental Quality
USEPA	United States Environmental Protection Agency
USEPA OSWER	USEPA Office of Solid Waste and Emergency Response
USEPA MCL	USEPA Maximum Contaminant Level
WHO	World Health Organization
WHO IPCS	International Programme on Chemical Safety (IPCS/INCHEM)
WHO IARC	International Agency for Research on Cancers
NA	Not Available.
NR	Not Relevant.

Toxicity terms:

BMC	Benchmark concentration
BMCL	Lower bound confidence limit on the BMC
BMD	benchmark dose
BMDL	Lower bound confidence limit on the BMD
CSF	Cancer slope Factor
CNS	Central nervous system
IURF or IUR	Inhalation unit risk factor
LOAEL	Lowest observed adverse effect level
LOEL	Lowest observed effect level
MRL	Minimal risk level (ATSDR)
NOAEL	No observed adverse effect level
NOEL	No observed effect level

RfC	Reference concentration
RfD	Reference dose
p-RfD	Provisional RfD
aRfD	Acute RfD
UF	Uncertainty factor
WOE	Weight of evidence

Section (C) Chemical-specific Absorption Factors

MDEQ	Michigan Department of Environmental Quality
USEPA RAGS-E	United States Environmental Protection Agency's Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment). July, 2004.

Section (D) Rule 57 Water Quality Values and GSI Criteria

GSI	Groundwater-surface water interface
NA	A value is not available or not applicable.
ID	Insufficient data to derive value
NLS	No literature search has been conducted

