



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Pyrene
CAS #:	129-00-0
Revised By:	RRD Toxicology Unit
Revision Date:	November 30, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	202.26	202.26	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	429	151.20	EPI	EXP
Boiling Point (°C)	404	404.00	EPI	EXP
Solubility (ug/L)	135	135	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.000004256	4.50E-06	EPI	EXP
HLC (atm-m ³ /mol at 25°C)	1.10E-5	1.19E-05	EPI	EXP
Log Kow (log P; octanol-water)	5.11	4.88	EPI	EXP
Koc (organic carbon; L/Kg)	1.06E+5	5.434E+04	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.0272	2.78E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	7.24E-6	7.25E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	NA	NA	NA	NA
Lower Explosivity Level (LEL; unitless)	NA	NA	NA	NA
Critical Temperature (K)		9.36E+02	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		1.44E+04	EPA2004	EXP
Density (g/mL, g/cm ³)		1.271	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	1.33E-07	3.85E-07	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	1.33E-07	3.85E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	1.57E-07	4.84E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	1.57E-07	4.84E-07	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	7.5E-2	3.0E-2	IRIS, 1993	
RfD details	<p>The IRIS RfD (3.0E-2) is based on a subchronic mouse oral study (USEPA, 1989). Male and female CD-1 mice (20/sex/group) were gavaged with 0, 75, 125, or 250 mg/kg/day pyrene in corn oil for 13 weeks. CRITICAL EFFECT = nephropathy and decreased kidney weights. NOAEL = 75 mg/kg-d. Total UF = 1,000 (10 each for intraspecies variability and interspecies and subchronic to chronic extrapolation. IRIS applied an addition UF = 3 for database deficiency that</p>	<p>Tier 1 Source: IRIS: Basis: The IRIS and PPRTV RfDs are the same and based on the same study. PPRTV refers to IRIS. Even though the PPRTV evaluation was conducted more recently than the IRIS evaluation, IRIS is selected as the best available value since it is a Tier 1 source. IRIS: RfD = 3.0E-2 mg/kg/day Critical Study: U.S. EPA. 1989. Mouse Oral Subchronic Toxicity of Pyrene. Study conducted by Toxicity Research Laboratories, Muskegon, MI for the Office of Solid Waste, Washington, DC. Methods: Male and female CD-1 mice (20/sex/group) were gavaged with 0, 75, 125, or 250 mg/kg/day pyrene in corn oil for 13 weeks. Critical effect: nephropathy (renal tubular pathology) and decreased kidney weights End point or Point of Departure (POD): NOEL = 75 mg/kg/day; LOAEL = 125 mg/kg/day. Uncertainty Factors: UF =3000; 10 each for intraspecies variability, interspecies extrapolation, and use of a subchronic study for chronic RfD derivation, and an additional 3 to account for the lack of both toxicity studies in a second species and developmental/reproductive studies. Source and date: IRIS; 7/1/1993</p> <p>Tier 2 Sources: PPRTV 9/5/2007: Sub chronic p-RfD = 3.0E-1 mg/kg/d; no chronic p-RfD provided in PPRTV. Chronic RfD = 3.0E-2 mg/kg/d. Sub chronic converted to chronic by MDEQ using additional 10x UF. Basis: PPRTV subchronic RfD based on IRIS (7/1/1993) Critical Study: U.S. EPA. 1989. Mouse Oral Subchronic Toxicity of Pyrene. Study conducted by Toxicity Research Laboratories, Muskegon, MI for the Office of Solid</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	was historically not applied by RD). The IRIS RfD was last revised: 7/1/1993.	<p>Waste, Washington, DC.</p> <p>Method: Male and female CD-1 mice (20/sex/group) were gavaged with 0, 75, 125, or 250 mg/kg/day pyrene in corn oil for 13 weeks.</p> <p>Critical effect: nephropathy and decreased kidney weights</p> <p>End point or Point of Departure (POD): NOAEL = 75 mg/kg/day</p> <p>Uncertainty Factors: UF = 3000; 10-fold for both intra- and intraspecies variability and 3 for the lack of both toxicity studies in a second species and developmental/reproductive studies; MDEQ applied an extra 10-fold UF for subchronic to chronic.</p> <p>MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD/RRD (1/15/1989), RfD = 7.5E-2 mg/kg/day. See Part 201 Value RfD details. *EPA used an additional 3-fold UF for lack of toxicity studies and reproduction studies in a second species. Per DEQ/WRD (7/28/1998), RfD = 2.5E-2 mg/kg-day based on a NOAEL of 75 mg/kg-day in a 90 day study of CD-1 mice (EPA, 1989) (3000--a 3-fold UF was used for database gaps since this was the only study available for pyrene).</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	No RD entry in EPB-CCD (9/16/11). Per IRIS: a quantitative estimate of the carcinogenic risk from oral exposure is not available at this	<p>Carcinogen Weight-of-Evidence (WOE) Class: Classification — D, not classifiable as to human carcinogenicity</p> <p>IRIS WOE Basis: Per PPRTV (2007); Not classifiable for human carcinogenicity based on no human data and inadequate data from animal experiments. No data are currently available and suitable for developing cancer values.</p> <p>Source and Date: PPRTV; 9/5/2007</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (1/1/1991), no value at this time. PPRTV: Per PPRTV (9/5/2007) no value at this time.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
	time (9/16/11). IRIS SF last revised: 1/1/91. No PPRTV p-OSF (1/4/12).	MRL: NA; MRLs are for non-cancer effects only. Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	1.0E+2	1.0E+2	MDEQ, 1993/NYDEC, 2006	
RfC/ITSL details	Per AQD: ITSL based on EPA RfD of 0.03 mg/kg. RfD based on NOAEL of 75 mg/kg for mice from 13 week gavage study EPA 1989. FINAL. AQD calculation date: 5/20/93.	Tier 3 Source: MDEQ and New York DEC: Basis: The IRIS and PPRTV RfCs are the same and are the only returned Tier values. See details below. Tier 1 and 2 Sources: IRIS: Per IRIS (9/1/1994), no value at this time. PPRTV: Per PPRTV (9/5/2007), no value at this time MRL: No MRL record available at this time. Tier 3 Sources: MDEQ: Per DEQ-CCD (AQD 1993), ITSL = $1.0\text{E}+2 \mu\text{g}/\text{m}^3$ based on route extrapolation of IRIS RfD of 0.03 mg/kg (see below): Critical Study: U.S. EPA. 1989. Mouse Oral Subchronic Toxicity of Pyrene. Study conducted by Toxicity Research Laboratories, Muskegon, MI for the Office of Solid Waste, Washington, DC Method: Male and female CD-1 mice (20/sex/group) were gavaged with 0, 75, 125, or 250 mg/kg/day pyrene in corn oil for 13 weeks. Averaging time = 24 hours. Critical effect: nephropathy and decreased kidney weights End point or Point of Departure (POD): NOAEL = 75 mg/kg/day Source and date: DEQ-CCD/AQD, 5/20/1993		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>New York DEC: Per NYDEC (2006), RfC= 1.0E+2 µg/m³ based on RfD of 0.03 mg/kg/day route extrapolation assuming a 70 kg adult and breathing rate of 20 m³ air/day.</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, Massachusetts, Minnesota, New Jersey and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m³)⁻¹)	--	NA	MDEQ, 2105	
IURF details	No AQD entry in EPB-CCD (9/16/11). No PPRTV p-IUR (1/4/12).	<p>Carcinogen Weight-of-Evidence (WOE) Class: Classification — D, not classifiable as to human carcinogenicity</p> <p>IRIS WOE Basis: Per PPRTV (2007); Not classifiable for human carcinogenicity based on no human data and inadequate data from animal experiments. No data is currently available and suitable for developing cancer values.</p> <p>Source and Date: PPRTV; 9/5/2007</p> <p>Tier 1 and 2 Sources:</p> <p>IRIS: Per IRIS (1/1/1991), no value at this time.</p> <p>PPRTV: Per PPRTV (9/5/2007) no value at this time.</p> <p>MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source:</p> <p>MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	
MMOA Details	--	NA		
		Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Developmental or Reproductive Effector? (Y/N)	No	No, the RfD is not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	NA		
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	
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	NA	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)	ID
Updated GSI value (µg/L)	ID
Rule 57 Drinking Water Value (µg/L)	15

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	15	7/1998
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	15	7/1998
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	NA	NA
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA	NA
Final Chronic Value (FCV)	ID	6/2001
Aquatic maximum value (AMV)	ID	6/2001
Final Acute Value (FAV)	ID	6/2001

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 ($\mu\text{g}/\text{kg}$)	330	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	5	MDEQ, 2015
Target Detection Limit – Air (ppbv)	1.20E+01	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	4.00E+02	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