



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Chrysene
CAS #:	218-01-9
Revised By:	RRD Toxicology Unit
Revision Date:	August 17, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	228.3	228.3	PP	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	523	258.20	PP	EXP
Boiling Point (°C)	448	448	PP	EXP
Solubility (ug/L)	1.6	2	PP	EXP
Vapor Pressure (mmHg at 25°C)	0.0000000076	6.23E-09	PP	EXP
HLC (atm-m³/mol at 25°C)	9.46E-5	5.23E-06	PP	EXP
Log Kow (log P; octanol-water)	5.7	5.81	PP	EXP
Koc (organic carbon; L/Kg)	4.01E+5	3.98E+05	SSG	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.0248	2.61E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	6.21E-6	6.7495E-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; unit less)	NA	NA	NA	NA
Critical Temperature (K)		9.79E+02	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		1.65E+04	EPA2004	EXP
Density (g/mL, g/cm ³)		1.274	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	8.37E-08	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	8.37E-08	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	1.03E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	1.03E-07	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Reference Dose (RfD) (mg/kg/day)	--	NA	MDEQ, 2015	
RfD details	NA	<p>Tier 1 and 2 Sources: IRIS: Per IRIS (12/01/1990), no value at this time. PPRTV: Per PPRTV (11/30/2001), no value at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 sources: MDEQ: Per DEQ-CCD, no value at this time.</p>		Complete
Oral Cancer Slope Factor (CSF) (mg/kg-day) ⁻¹	4.1E-3	1.0E-3	USEPA, 1993/IRIS, 2014	
CSF details	Based on CSF for benzo (a) pyrene and a relative potency of 0.001. Source: IRIS/ERD CCD date: 3/21/2000	<p>Tier 1 Source: USEPA/IRIS Basis: The CSF for chrysene is derived by applying a toxicity equivalency factor (TEF) of 0.001 for Chrysene to the recommended CSF for benzo[a]pyrene = 1.0 per mg/kg-day based on the alimentary tract tumor response in female B6C3F1 mice (IRIS Toxicological Review of Benzo[a]pyrene External Review Draft, 12/2014). U.S. EPA Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons (EPA/600/R-93/089, July 1993) recommends that a toxicity equivalency factor (TEF) be used to convert concentrations of carcinogenic polycyclic aromatic hydrocarbons (cPAHs) to an equivalent concentration of benzo (a) pyrene (BaP) when assessing the cancer risks posed by these substances from oral exposures. These TEFs are based on the potency of each compound relative to that of BaP. The TEF of chrysene is 0.001.</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: B2; probable human carcinogen IRIS WOE Basis: based on development of carcinomas and malignant lymphoma in mice after intraperitoneal injection, skin carcinomas in mice following dermal exposure, and chromosomal abnormalities in hamsters and mouse germ cells after gavage exposure. Positive responses in bacterial gene mutation assays and transformed mammalian cells exposed in culture have been observed. Chrysene is</p>		Complete

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>a component of PAH mixtures that have been associated with human cancer. Source and Date: PPRTV, 11/30/2001</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (12/01/1990), no value at this time. An IRIS Toxicological Review of Benzo[a]pyrene was released for external peer review in September 2014. CSF is based on CSF for benzo (a) pyrene. See details above. PPRTV: Per PPRTV (11/30/2001), no value at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD/RRD (3/21/2000), CSF = 4.1E-3 (mg/kg-day)⁻¹ Basis: based on CSF for benzo (a) pyrene (4.1E+0 per mg/kg-day) and application of a toxicity equivalency factor (TEF) of 0.001. Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons (EPA/600/R-93/089, July 1993), recommends that a TEF be used to convert concentrations of carcinogenic polycyclic aromatic hydrocarbons (cPAHs) to an equivalent concentration of benzo (a) pyrene (BaP) when assessing the cancer risks posed by these substances from oral exposures. These TEFs are based on the potency of each compound relative to that of BaP.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	--	NA	MDEQ, 2015	
RfC/ITSL details	NA	<p>Tier 1 and 2 Sources: IRIS: Per IRIS (12/01/1990), no value at this time. PPRTV: Per PPRTV (11/30/2001), no value 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



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$) ⁻¹)	--	6.0E-7	USEPA, 1993/IRIS, 2014	
IURF details	<p>A review of available literature did not produce any studies that could be used to do a quantitative risk assessment. IRSL/SRSL is not being calculated at this time (Aug 26, 1993). There are many positive dermal and injection carcinogenicity studies. The potency for chrysene is expected to be less than that for benzo (a) pyrene. Thus, any ambient impact less than the B (a) P number would not be of concern. Use SAP's 7-20-95 advisory on how to calculate</p>	<p>Tier 1 Source: USEPA/IRIS: Basis: The IURF for chrysene is derived by applying a toxicity equivalency factor (TEF) of 0.001 for Chrysene to the recommended IURF for benzo[a]pyrene = 6.0E-4 per $\mu\text{g}/\text{m}^3$ (IRIS Toxicological Review of Benzo[a]pyrene External Review Draft, 12/2014). U.S. EPA Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons (EPA/600/R-93/089, July 1993) recommends that a TEF be used to convert concentrations of carcinogenic polycyclic aromatic hydrocarbons (cPAHs) to an equivalent concentration of benzo (a) pyrene (BaP) when assessing the cancer risks posed by these substances from oral exposures.</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: B2; probable human carcinogen IRIS WOE Basis: based on development of carcinomas and malignant lymphoma in mice after intraperitoneal injection, skin carcinomas in mice following dermal exposure, and chromosomal abnormalities in hamsters and mouse germ cells after gavage exposure. Positive responses in bacterial gene mutation assays and transformed mammalian cells exposed in culture have been observed. Chrysene is a component of PAH mixtures that have been associated with human cancer. Source and Date: PPRTV, 11/30/2001</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (12/01/1990), no value at this time. An IRIS Toxicological Review of Benzo[a]pyrene was released for external peer review in September 2014. IURF is based on IURF for benzo (a) pyrene. See details above. PPRTV: Per PPRTV (11/30/2001), no value at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD/AQD (7/20/1995), IURF = 2.1E-6 ($\mu\text{g}/\text{m}^3$)⁻¹ Basis: based on IURF for benzo (a) pyrene (2.1E-3) and application of a toxicity</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
	screening level using TEF methodology. CCD/AQD date: 7/20/1995.	equivalency factor (TEF) of 0.001. Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons (EPA/600/R-93/089, July 1993), recommends that a TEF be used to convert concentrations of carcinogenic polycyclic aromatic hydrocarbons (cPAHs) to an equivalent concentration of benzo (a) pyrene (BaP) when assessing the cancer risks posed by these substances from oral exposures.		
Mutagenic Mode of Action (MMOA)? (Y/N)	--	YES	USEPA, 2015	
MMOA Details	--	Listed as a carcinogen with mutagenic MOA in the EPA OSWER List.		
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) (ug/L)	--	NO	SDWA, 1976	
SDWS details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399.		
Secondary Maximum Contaminant Level (SMCL) (ug/L)	--	NO	SDWA, 1976 and USEPA SMCL List, 2015	
SMCL details	NA	SDWA, 1976 and USEPA SMCL List, 2015		
Is there an aesthetic value for drinking water? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value (ug/L)	NA	NA	NA	
Aesthetic Value details	NA	NA		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	NA	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)	---	0.13	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)	ID

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	ID	3/1999
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	ID	3/1999
Wildlife Value (WV)	NA	NA
Human Cancer Values for Drinking Water Source (HCV-drink)	ID	3/1999
Human Cancer values for non-drinking water source (HCV-Non-drink)	ID	3/1999
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 ($\mu\text{g}/\text{L}$)	1	MDEQ, 2015
Target Detection Limit – Air (ppbv)	NA	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	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