



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Gentian violet
CAS #:	548-62-9
Revised By:	RRD Toxicology Unit
Revision Date:	September 21, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	408	407.99	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	---	215.00	EPI	EXP
Boiling Point (°C)	---	NA	NA	
Solubility (ug/L)	1.00E+6	4000000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	1.93E-14	1.93E-14	PP	EST
HLC (atm-m ³ /mol at 25°C)	3.06E-16	3.06E-16	PP	EST
Log Kow (log P; octanol-water)	0.51	0.96	EPI	EXP
Koc (organic carbon; L/Kg)	3.17	6.711E+05	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.08	3.45E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	8.0E-6	4.04E-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)		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	4.43E-13	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	4.43E-13	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	4.43E-13	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	4.43E-13	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.4E-1	1.4E-1	MDEQ, 1990	
RfD details	<p>Mouse chronic dietary study (Littlefield et al., 1985); NOEL = 100ppm (14.28 mg/kg/day); UF = 100; Critical effects = increased mortality, erythropoiesis in spleen & atrophy of the ovaries. CCD/RRD date: 6/26/1990 CCD/SWQD date - 3/21/1990.</p>	<p>Tier 3 Source: MDEQ: Basis: MDEQ value based on a chronic toxicity and carcinogenicity study (Littlefield et al. 1985). No value is available from other Tier 3 sources. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS files for gentian violet available at this time. PPRTV: No PPRTV record for gentian violet is available at this time. MRL: No MRL record for gentian violet is available at this time.</p> <p>Tier 3 Sources: MDEQ/RRD (06/26/1990); RfD = 1.4E-1 mg/kg-day Critical Study: Littlefield NA, et al. (1985) Chronic toxicity and carcinogenicity studies of gentian violet in mice. Fundam Appl Toxicol. 5(5):902–12. Method(s): 720 male and 720 female B6C3F1 mice (4–5 weeks old) were fed gentian violet (99% gentian violet and 1% methyl violet) at dietary concentrations of 0, 100, 300, or 600 mg/kg feed (equivalent to 0, 10.7–14.3, 32.1–35.7 and 64.3 mg/kg bw/day for males and 0, 14.3, 35.7–39.3 and 71.4 mg/kg bw/day for females, respectively). Critical effect: increased mortality, erythropoiesis in spleen and atrophy of the ovaries End point or Point of Departure (POD): NOAEL = 100 ppm (14.3 mg/kg/day) in female mice. Uncertainty Factors: UF = 100 (10 each for interspecies variability and interspecies extrapolation) Source and date: MDEQ-CCD/RRD, 6/26/1990, and WRD, 3/21/1990.</p> <p>OTHERS: No value is available at this time from these Tier 3 sources/databases:</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		HEAST, NTP ROC, health and environmental agencies of California, Massachusetts, Minnesota, New Jersey, New York, and Texas, Canada, The Netherlands (RIVM), WHO (IARC), WHO (IPCS/INCHEM), ECHA (REACH) and OECD HPV.		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	5.5E-2	5.5E-2	MDEQ, 2000	
CSF details	<p>Mouse chronic dietary study (Littlefield et al., 1985). Liver tumors in female mice. Carcinogenic potential not classified by EPA. CCD/RRD date: 3/10/2000. Per CCD/WRD, 3/10/1990. CSF = 5.5E-2. Hepatocellular neoplasms in female B6C3F1 mice exposed via the diet for 2 years (Littlefield, 1985).</p>	<p>Tier 3 Source: MDEQ: Basis: MDEQ value based on a chronic toxicity and carcinogenicity study (Littlefield et al. 1985, 1989). No value is available from other Tier 3 sources. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS files for gentian violet available at this time. PPRTV: No PPRTV record for gentian violet available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ/RRD (03/10/2000); CSF = 5.5E-2 (mg/kg-day)⁻¹ Critical Studies: 1) Littlefield NA, et al. (1985) Chronic toxicity and carcinogenicity studies of gentian violet in mice. <i>Fundam Appl Toxicol.</i> 5(5):902–12. 2) Littlefield NA, et al. (1989). Chronic toxicity/carcinogenicity studies of gentian violet in Fischer 344 rats: two-generation exposure. <i>Food Chem Toxicol.</i> 27:239–47. Method(s): 720 male and 720 female B6C3F1 mice (4–5 weeks old) were fed gentian violet at dietary concentrations of 0, 100, 300, or 600 mg/kg feed (Littlefield et al., 1985). 1) <i>Dose response data: Tumor Type</i> – hepatocellular tumors; <i>Test Species</i> – female mice; <i>Route</i> - oral (diet) 2) <i>Extrapolation method:</i> linearized multistage model Source and date: MDEQ-CCD/RRD, 03/10/2000</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>OTHERS: 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, New York, and Texas, Canada, The Netherlands (RIVM), WHO (IARC), WHO (IPCS/INCHEM), ECHA (REACH) and OECD HPV.</p> <p>Carcinogen Weight-of-Evidence (WOE) Class: Genotoxic and carcinogenic (class is not specified)</p> <p>WOE Basis: multisite carcinogen in mouse and rat species. Committee noted that there is inadequate information to determine the overall carcinogenicity of the metabolites of gentian violet (demethylated gentian violet, leucogentian violet and its demethylated metabolites):</p> <ol style="list-style-type: none"> 1) There is a published report that one of the possible metabolites of gentian violet, demethylated leucopararosaniline, is carcinogenic in rats, but no information is available on its potency. 2) There is no information on the carcinogenicity of the major metabolite, leucogentian violet. The structure of gentian violet is similar to that of malachite green, and it is known that leucomalachite green is a more potent carcinogen than malachite green; therefore, it is possible that leucogentian violet is similarly a more potent carcinogen than gentian violet. 3) Gentian violet and leucogentian violet are readily interconvertible in the body, and so it is likely that exposure to gentian violet will also result in exposure to leucogentian violet. <p>Source and date: WHO (2014). WHO Food Additive Series: 69. Toxicological evaluation of certain veterinary drug residues in food. JECFA, WHO.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	--	NA	MDEQ, 2015	
RfC/ITSL details	NA	<p>Tier 1 and 2 Sources:</p> <p>IRIS: No IRIS files for gentian violet available at this time.</p>		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>PPRTV: No PPRTV record for gentian violet available at this time. MRL: No MRL record for gentian violet available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no inhalation toxicity value for gentian violet at this time.</p>		
Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$) ⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Tier 1 and 2 Sources: IRIS: No IRIS files for gentian violet available at this time. PPRTV: No PPRTV record for gentian violet available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no inhalation toxicity value for gentian violet 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	NO	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	The RfD is not based on a reproductive-developmental effect.		
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	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
SMCL details	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 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		
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)	---	0.1	MDEQ, 2015	
AE _d details				
Ingestion Absorption Efficiency (AE _i)		1.0	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)	NA
Rule 57 Drinking Water Value (µg/L)	NA

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

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
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