



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Diquat
CAS #:	85-00-7
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)	344.08	344.05	EPI	EXP
Physical State at ambient temp	Solid	Solid	MDEQ	
Melting Point (°C)	---	337	PP	EXP
Boiling Point (°C)	---	NA	NA	
Solubility (ug/L)	7.00E+5	7.07900E+08	PP	EXP
Vapor Pressure (mmHg at 25°C)	0.00000181	1.81E-06	PP	EST
HLC (atm-m³/mol at 25°C)	1.42E-13	1.42E-13	PP	EST
Log Kow (log P; octanol-water)	-2.82	-4.60	PP	EXP
Koc (organic carbon; L/Kg)	0.00169	NA	NA	NA
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.08	2.08E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	8.0E-6	5.1922E-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)		NA	NA	NA
Enthalpy of Vaporization (cal/mol)		NA	NA	NA
Density (g/mL, g/cm ³)		1.24	CRC	EXP
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)	2.2E-03	5.0E-3	OPP, 2009	
RfD details	Chronic, in-feed, rat study. UF=100, NOAEL=0.22 mg/kg/d; Critical effect = minimal lens opacity & cataracts (Chevron, chem 1985). CCD date: 7/22/1986	<p>Tier 1 Source: EPA-OPP: Basis: RfD = 0.005 mg/kg/day. OPP value is best available data because it is the most current documentation. Critical Study: Hopkins MN (1990). Diquat: one year feeding study in dogs. ICI Study No. CTL/P/2596. DPR Vol. 226-094 (MRID 41730301) Methods: Groups of 4 male and 4 female beagle dogs were administered technical grade diquat dibromide in the diet for 52 weeks. Male dogs received daily 400 g and females 350 g of the diquat-containing pellets. The dose levels used were 0, 0.5, 2.5 or 12.5 mg/kg/day, expressed as diquat cation, and were based on the results of previous toxicity studies with diquat dibromide (details were not provided). Critical effect: unilateral cataracts in females and decreased weight of the epididymides in males End point or Point of Departure (POD): systemic NOAEL (both sexes) = 0.5 mg/kg/day Uncertainty Factors: UF = 100 (10 for each inter- and interspecies variability) Source and date: EPA-OPP Reregistration Eligibility Decision (RED) Diquat Dibromide EPA 738-R-95-016 (July 1995); EPA-OPP Memo Diquat dibromide: Human health risk scoping document in support of registration review (Dec 2, 2009). IRIS: RfD = 2.2E-03 mg/kg/day Critical Study: Chevron Chemical Company. 1985. MRID No. 00145855, 00155474, 00160673. Available from EPA. Write to FOI, EPA, Washington, DC 20460. (unpublished) Methods: Sprague-Dawley rats (50/sex/dose) were fed 0, 5, 15, 75, or 375 ppm of diquat in diets for 2 years. Doses were expressed in terms of diquat cation and reported as ppm in the diet and as mg/kg bw/day.</p>	OPP, 2009	Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Critical effect: lens opacity and eye cataracts End point or Point of Departure (POD): NOAEL = 0.22 mg/kg/day Uncertainty Factors: UF = 100 (10 each for interspecies variability and interspecies extrapolation) Source and date: IRIS, Last revision date - 1/01/1995. An EPA screening-level review in 2001 identified one or more significant new studies.</p> <p>Tier 2 Sources: 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, RRD adopted IRIS value.</p>		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	NA	<p>Weight of Evidence: Group E chemical; evidence of non-carcinogenicity for humans Source and date: EPA-OPP Reregistration Eligibility Decision (RED) Diquat Dibromide EPA 738-R-95-016 (July 1995); EPA-OPP Memo Diquat dibromide: Human health risk scoping document in support of registration review (Dec 2, 2009).</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (1/01/1995), no value at this time. No cancer assessment information is available. 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>		Complete
Reference Concentration	--	NA	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
(RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)				
RfC/ITSL details	NA	<p>Tier 1 and 2 Sources: IRIS: Per IRIS (1/01/1995), no value at this time. No cancer assessment information is available. 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	MDEQ, 2015	
IURF details	NA	<p>Weight of Evidence: Group E chemical; evidence of non-carcinogenicity for humans Source and date: EPA-OPP Reregistration Eligibility Decision (RED) Diquat Dibromide EPA 738-R-95-016 (July 1995); EPA-OPP Memo Diquat dibromide: Human health risk scoping document in support of registration review (Dec 2, 2009).</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (1/01/1995), no value at this time. No cancer assessment information is available. 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>		Complete
Mutagenic Mode of Action (MMOA)? (Y/N)	--	NO	USEPA, 2015	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
MMOA Details	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
Developmental or Reproductive Effector? (Y/N)	No	No. The RfD is based on two critical effects one of which is a reproductive-developmental effect. MDEQ does not consider this substance a developmental toxicant at this time.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	Critical Study: Hopkins MN (1990). Diquat: one year feeding study in dogs. ICI Study No. CTL/P/2596. DPR Vol. 226-094 (MRID 41730301) Methods: Groups of 4 male and 4 female beagle dogs were administered technical grade diquat dibromide in the diet for 52 weeks. Male dogs received daily 400 g and females 350 g of the diquat-containing pellets. The dose levels used were 0, 0.5, 2.5 or 12.5 mg/kg/day, expressed as diquat cation, and were based on the results of previous toxicity studies with diquat dibromide (details were not provided). Critical effect: unilateral cataracts in females and decreased weight of the epididymides in males		
State Drinking Water Standard (SDWS) (ug/L)	--	20	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	
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	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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)	20 (M); 6.0
Updated GSI value (µg/L)	20 (M); 6.0
Rule 57 Drinking Water Value (µg/L)	61

NUMBERS IN TABLE COME FROM CAS # 2764729

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	61	12/2002
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	4,900	12/2002
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)	6.0	7/2011
Aquatic maximum value (AMV)	54	7/2011
Final Acute Value (FAV)	110	7/2011

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 ($\mu\text{g}/\text{L}$)	20	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