



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Dinoseb (DD)
CAS #:	88-85-7
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)	240.2	240.22	EPI	EXP
Physical State at ambient temp	Liquid	Solid	MDEQ	
Melting Point (°C)	313	40.00	EPI	EXP
Boiling Point (°C)	---	332.00	EPI	EXP
Solubility (ug/L)	52000	52000	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.07524	5.25E-05	PC	EXP
HLC (atm-m ³ /mol at 25°C)	4.60E-7	4.56E-07	PP	EST
Log Kow (log P; octanol-water)	3.15	3.56	EPI	EXP
Koc (organic carbon; L/Kg)	1250	4294	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm ² /s)	0.08	4.92E-02	W9	EST
Diffusivity in Water (Dw; cm ² /s)	8.0E-6	5.7449E-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	15.6	PC	EXP
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)		NA	NA	NA
EMSOFT Flux Residential 2 m (mg/day/cm ²)	NA	4.50E-07	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	NA	4.50E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	NA	5.66E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	NA	5.66E-07	EMSOFT	EST

(B) Toxicity Values/Benchmarks

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.0E-3	1.0E-3	IRIS, 1989	
RfD details	<p>Rat 3-year reproduction dietary study (Dow Chemical Co., 1981); NOAEL = none; LOAEL = 1mg/kg/day; UF = 1000; Critical effect is decreased fetal weight. Source: IRIS CCD/RRD date: 12/9/1986</p>	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. IRIS (1989) RfD = 1.0E-3 mg/kg-day: Critical Study: 3-Generation Reproductive Study, Dow Chemical Co. 1981a. MRID No. 00152675. (Unpublished). [Irvine L, Armitage A (1981). 2-secbutyl-4,6-dinitrophenol (Dinoseb): Three generation reproductive performance study in the rat (dietary). Hazelton Laboratories Europe, Ltd. Prepared for Agricultural Chemical, Dow Chemical Pacific, Ltd., Hong Kong. U.S. EPA Accession No. 259399] Methods: Rats (25/sex/dose; 2 littering groups/generation) were exposed to 0, 1, 3, and 10 mg/kg bw/day dinoseb in their diet for 29 weeks. Critical effect: decreased fetal weight End point or Point of Departure (POD): LEL = 1 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for interspecies variability, interspecies extrapolation, and of NOEL) Source and date: IRIS, Last revision date - 8/01/1989. An IRIS screening-level review in 2003 identified one or more significant new studies pertinent to the RfD.</p> <p>Tier 2 Sources: PPRTV: Per PPRTV (May 31, 2002), no value at this time. The 2002 PPRTV evaluated only the carcinogenic potential of dinoseb. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: 1) Per DEQ-CCD (12/9/1986), RRD adopted the IRIS RfD. See Part 201 RfD details. 2) Per DEQ-CCD (5/1/2000), WRD RfD = 1.0E-3 mg/kg-day based on a LOAEL of 1 mg/kg-day for depressed pup weight gain during the lactation period. The critical study is a three-generation study in rats (Irvine and Armitage, 1981). The total UF</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		is 1000 (10 each for interspecies variability, interspecies extrapolation, and use of LOAEL). Critical study: Irvine L, Armitage A (1981). 2-secbutyl-4,6-dinitrophenol (Dinoseb): Three generation reproductive performance study in the rat (dietary). Hazelton Laboratories Europe, Ltd. Prepared for Agricultural Chemical, Dow Chemical Pacific, Ltd., Hong Kong. U.S. EPA Accession No. 259399		
Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹	--	NA	MDEQ, 2015	
CSF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: D; not classifiable as to human carcinogenicity (IRIS, 1993)</p> <p>WOE Basis: Dinoseb was not carcinogenic in two inadequate studies in rats and in mice. In a third study, an increase in benign liver tumors in female mice was not considered to be treatment-related. (IRIS, 1993)</p> <p>Per PPRTV (2002):</p> <p>1) Case-control studies in Swedish cancer patients, described in U.S. EPA (1984), found no evidence of increased risk of malignant lymphomas or malignant mesenchymal soft tissue tumors associated with dinoseb exposure (Eriksson et al., 1979; Hardell et al., 1981).</p> <p>2) Long-term studies of dinoseb exposure in mice (Innes et al., 1969; Dow Chemical Co., 1981) and rats (Dow Chemical Co., 1977) did not show an increase in tumors and/or were inadequate studies of carcinogenicity (U.S. EPA, 1984, 2001). No additional studies subsequent to the 1989 IRIS review were located.</p> <p>3) Genotoxicity assays of dinoseb have generally shown no mutagenic activity, but have demonstrated an ability to interact with DNA and RNA (U.S. EPA, 1984, 2001).</p> <p>Source and Date: PPRTV, 5/31/2002; IRIS, Last revision date - 7/01/1993. An IRIS screening-level review in 2003 did not identify any critical new studies relating to cancer assessment.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (7/01/1993), no value at this time. PPRTV: Per PPRTV (5/31/2002), no value at this time due to lack of data.</p>	Complete	

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<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>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ($\mu\text{g}/\text{m}^3$)	0.1	4.0E+0	MDEQ, 2004	
RfC/ITSL details	Due to a lack of available toxicity information ITSL based on default value, from R232(1)(i). CCD/AQD date: 10/17/2003	<p>Tier 3 Source:</p> <p>MDEQ:</p> <p>Basis: MDEQ value based on extrapolated IRIS oral RfD from a 3-generation reproductive study. ECHA (REACH) using the same approach and key study as MDEQ chose a different critical effect (and a NOAEL) and applied a lower UF. See details below.</p> <p>Tier 1 and 2 Sources:</p> <p>IRIS: Per IRIS (12/09/1986), no value at this time.</p> <p>PPRTV: Per PPRTV (5/31/2002), no value at this time.</p> <p>MRL: No MRL record available at this time.</p> <p>Tier 3 Sources:</p> <p>MDEQ: AQD (2004) ITSL = 4.0E+0 $\mu\text{g}/\text{m}^3$. Averaging time = 24 hours.</p> <p>Basis: based on the IRIS (1989) RfD of 0.001 mg/kg/day and assumption of 70 kg body weight and 20m³/day inhalation rate:</p> <p>Critical Study: 3-Generation Reproductive Study, Dow Chemical Co. 1981a. MRID No. 00152675. (Unpublished). [Irvine L, Armitage A (1981). 2-secbutyl-4,6-dinitrophenol (Dinoseb): Three generation reproductive performance study in the rat (dietary). Hazelton Laboratories Europe, Ltd. Prepared for Agricultural Chemical, Dow Chemical Pacific, Ltd., Hong Kong. U.S. EPA Accession No. 259399]</p> <p>Methods: Rats (25/sex/dose; 2 littering groups/generation) were exposed to 0, 1, 3, and 10 mg/kg bw/day dinoseb in their diet for 29 weeks.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>Critical effect: decreased fetal weight End point or Point of Departure (POD): LOAEL = 1 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for interspecies variability, interspecies extrapolation, and lack of NOEL) Source and date: IRIS, Last revision date - 8/01/1989; DEQ-CCD/AQD 3/19/2004</p> <p>ECHA: Derived No Effect Level (DNEL) = 0.01 mg/m³ (1.0E+1 µg/m³) derived as follows: Key study: Study report, 1981 [3-Generation Reproductive Study, Dow Chemical Co. 1981a. MRID No. 00152675. (Unpublished). Method: 3 generation reproduction study; Groups of Sprague-Dawley rats (25/sex/dose) in each of the 3 generations (F0, F1 and F2) received Dinoseb in the diet at concentrations to provide 1, 3 or 10 mg/kg bw daily for 29 weeks (total duration 87 weeks). Similar groups of animals-fed untreated diet over the same period served as the control group. The parents of all 3 generations were fed the appropriate diets for 13 weeks and then subjected to 2 mating trials. The offspring from the first mating of each parental generation (F1a, F2a and F3a) were maintained until weaning and then killed and necropsied. A proportion of the parental females from each group and generation were killed on day 21 after the second mating for teratological observation. Critical effect: reduction in the body weight and appearance of a yellowish tinge in the fur. NOAEL: 3 mg/kg-day Dose descriptor starting point (after route to route extrapolation): NOAEC - 0.25 mg/m³ Overall assessment factor (AF): 25 AF for other interspecies differences: 2.5 AF for interspecies differences: 10 Source: ECHA REACH Dossier for Dinoseb, 2015</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</p>		

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		California, Massachusetts, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), and OECD HPV.		
Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$) ⁻¹)	--	NA	MDEQ, 2015	
IURF details	NA	<p>Carcinogen Weight-of-Evidence (WOE) Class: D; not classifiable as to human carcinogenicity (IRIS, 1993)</p> <p>WOE Basis: Dinoseb was not carcinogenic in two inadequate studies in rats and in mice. In a third study, an increase in benign liver tumors in female mice was not considered to be treatment-related. (IRIS, 1993)</p> <p>Per PPRTV (2002):</p> <p>1) Case-control studies in Swedish cancer patients, described in U.S. EPA (1984), found no evidence of increased risk of malignant lymphomas or malignant mesenchymal soft tissue tumors associated with dinoseb exposure (Eriksson et al., 1979; Hardell et al., 1981).</p> <p>2) Long-term studies of dinoseb exposure in mice (Innes et al., 1969; Dow Chemical Co., 1981) and rats (Dow Chemical Co., 1977) did not show an increase in tumors and/or were inadequate studies of carcinogenicity (U.S. EPA, 1984, 2001). No additional studies subsequent to the 1989 IRIS review were located.</p> <p>3) Genotoxicity assays of dinoseb have generally shown no mutagenic activity, but have demonstrated an ability to interact with DNA and RNA (U.S. EPA, 1984, 2001).</p> <p>Source and Date: PPRTV, 5/31/2002; IRIS, Last revision date - 7/01/1993. An IRIS screening-level review in 2003 did not identify any critical new studies relating to cancer assessment.</p> <p>Tier 1 and 2 Sources: IRIS: Per IRIS (7/01/1993), no value at this time. PPRTV: Per PPRTV (5/31/2002), no value at this time due to lack of data. 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	



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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. http://www.epa.gov/oswer/riskassessment/sghandbook/chemicals.htm		
Developmental or Reproductive Effector? (Y/N)	Yes	YES- for both oral and inhalation, the RfD and RfC are based on a reproductive-developmental effect. Oral Exposure Pathways-Full Term Exposure Inhalation Exposure Pathways- Full Term Exposure	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	NA	Reproductive effect: decreased fetal weight Reproductive Study: 3-Generation Reproductive Study, Dow Chemical Co. 1981a. MRID No. 00152675. (unpublished)		
State Drinking Water Standard (SDWS) (ug/L)	7.0	7.0	SDWA, 1976	
SDWS details	SDWA, 1976	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	
Aesthetic Value details	NA	NA		
Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	NA	NA	NA	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
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)	1.0 (M); 0.48
Updated GSI value (µg/L)	1 (M,X); 0.48
Rule 57 Drinking Water Value (µg/L)	28

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	28	6/2000
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	1,900	6/2000
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)	0.48	5/2000
Aquatic maximum value (AMV)	4.8	5/2000
Final Acute Value (FAV)	9.5	5/2000

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 ($\mu\text{g}/\text{kg}$)	200	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