



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>2,6-Dichloro-4-nitroaniline</b>
<b>CAS #:</b>	<b>99-30-9</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	August 17, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
<b>Molecular Weight (g/mol)</b>	207.02	207.02	EPI	EXP
<b>Physical State at ambient temp</b>	Solid	Solid	MDEQ	
<b>Melting Point (°C)</b>	---	191.00	EPI	EXP
<b>Boiling Point (°C)</b>	---	NA	NA	
<b>Solubility (ug/L)</b>	7000	7E+03	EPI	EXP
<b>Vapor Pressure (mmHg at 25°C)</b>	0.0000012	1.20E-06	EPI	EXP
<b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>	4.67E-8	4.67E-08	PP	EST
<b>Log Kow (log P; octanol-water)</b>	2.76	2.80	EPI	EXP
<b>Koc (organic carbon; L/Kg)</b>	517	1947	EPI	EST
<b>Ionizing Koc (L/kg)</b>		NR	NA	NA
<b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>	0.08	1.30E-02	W9	EST
<b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>	8.0E-6	2.8838E-06	W9	EST

	Part 201 Value	Updated Value	Reference Source	Comments
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA
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 <sup>3</sup> )		0.28	PC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	NA	9.66E-08	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	NA	9.66E-08	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	NA	1.18E-07	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	NA	1.18E-07	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
<b>Reference Dose (RfD) (mg/kg/day)</b>	3.0E-1	2.5E-3	USEPA-OPP, 2006	
<b>RfD details</b>	80 week in feed mouse study; NOAEL = 30mg/kg-d; UF = 100; Critical effect = hepatotoxicity (Mallyon & Marhum, 1989). CCD/RRD date: 8/23/94	<p><b>Tier 1 Source:</b>  <b>USEPA-OPP:</b>  <b>Basis:</b> OPP is a Tier 1 source. USEPA-OPP (2006) chronic population adjusted dose (cPAD) = 0.0025 (2.5E-3) mg/kg-day.  <b>EPA/OPP:</b>  <b>Critical Study:</b> Killeen, J. (2002) A 52-Week Oral Toxicity Study in Dogs with Dicloran: Lab Project Number: 012260-1. Unpublished study prepared by Ricerca, LLC. 329 p. (MRID 45610801)  <b>Methods:</b> One-year chronic toxicity study in dogs  <b>Critical effect:</b> clinical chemistry effects (increased alkaline phosphatase in both sexes and increased cholesterol in males), increased liver weights, hepatocyte hypertrophy, vacuolar alterations of the brain and spinal cord, <b>prostate atrophy, degeneration of the seminiferous tubules, and hypospermia in the epididymides</b>  <b>End point or Point of Departure (POD):</b> NOAEL = 2.5 mg/kg-day  <b>Uncertainty Factors:</b> UF = 1000 (10 each for intraspecies variability and interspecies extrapolation and 10x FQPA Safety Factor)  <b>Additional Note:</b>                      OPP used a rat developmental study (MRID 46447501) to assess risks for the population group of females 13-49 years of age. A developmental study is appropriate for assessing acute risks because developmental effects are presumed to occur as a result of a single dose at a critical time during gestation. The developmental NOAEL of 50 mg/kg/day was based on increased incidences of supernumerary rudimentary ribs and also decreased fetal weights at 100 mg/kg/day. Applying a UF of 1000, the <b>acute aPAD = 0.05 (5.0E-2)</b> mg/kg-day.  <b>Source and date:</b> EPA/OPP Reregistration Eligibility Decision (RED) for DCNA (Dicloran), 6/14/2006. IRIS refers to EPA-OPP for updated assessments of pesticides.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available at this time.  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> CCD/RRD (1994) RfD = 3.0E-1 mg/kg-day:  <b>Critical Study:</b> Mallyon, B.A. &amp; Markham, L.P. (1989) Technical dicloran: Oncogenicity study in the mouse. Unpublished report No. TOX/86006 from Schering Agrochemicals Ltd, United Kingdom. Submitted to WHO by Gowan Company, Yuma, Arizona, USA.  <b>Method(s):</b> 80-week DCNA in feed mouse study  <b>Critical effect:</b> hepatotoxicity  <b>End point or Point of Departure (POD):</b> NOAEL = 30 mg/kg-day  <b>Uncertainty Factors:</b> UF = 100 (10 each for intraspecies variability and interspecies extrapolation)  <b>Source and date:</b> MDEQ-CCD/RRD, 8/3/1994</p>		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day<sup>-1</sup>)</b>	--	NA	MDEQ, 2015	
<b>CSF details</b>	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> CARC classified Dicloran as "Suggestive Evidence of Carcinogenic Potential"  <b>WOE Basis:</b> based on benign testicular Leydig cell tumors in male rats (1 sex, 1 species) at the high dose, which was considered adequate but not excessive, as well as a positive Ames test. In addition, there is some evidence that a plant metabolite, but not an animal metabolite, had some carcinogenic activity. No evidence of carcinogenicity was seen in mice at doses that were considered to be adequate for the assessment of carcinogenicity of dicloran.  <b>Source and Date:</b> EPA/OPP (9/5/2006) Memorandum: DICLORAN: Report of the Cancer Assessment Review Committee (CARC) PC Code: 031301 (Evaluation of the Carcinogenic Potential of Dicloran), TRX No. 0054321</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available at this time.  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD, no value at this time.</p>		
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ( $\mu\text{g}/\text{m}^3$ )	--	8.8E+0	USEPA-OPP, 2006; MDEQ, 2015	
RfC/ITSL details	NA	<p><b>Tier 1 Source:</b>  <b>USEPA-OPP:</b>  <b>Basis:</b> EPA-OPP (2006) an intermediate term (1-6 months) occupational level of concern (LOC)/margin of exposure (MOE) of 100 based on NOAEL = 2.5 mg/kg/day and UF = 100. MDEQ applied an additional UF of 10 to account for subchronic to chronic extrapolation, MDEQ derived an <b>RfC = 0.00875 mg/m<sup>3</sup></b> based on OPP data and assuming 70 kg body weight and 20 m<sup>3</sup>/day inhalation rate:  <math>\text{RfC} = 2.5 * (70/20) / 1000 = 8.75 \mu\text{g}/\text{m}^3</math>.</p> <p><b>EPA/OPP:</b>  <b>Critical Studies:</b>                      1) Woodard, G.; Cronin, M.T.I. (1962) U-2069: Interim Report (13 Weeks): Safety Evaluation by Oral Administration to Rats and Dogs for 104 Weeks. (Unpublished study received Jun 1, 1963 under PP0375; prepared by Woodard Research Corp., submitted by Upjohn Co., Kalamazoo, Mich.; CDL:090404-Z) (MRIDs 29056)                      2) Kakuk, T.J.; Weddon, T.W.; Thomas, R.W.; et al. (1979) Reevaluation of Potential Hepatic Effects of Botran in Beagle Dogs--Supplemental Report: Technical Report No. 001-9610-79-005. (Unpublished study received Dec 19, 1979 under 1023-51; prepared in cooperation with Woodward Research Corp., submitted by Upjohn Co., Kalamazoo, Mich.; CDL:241511-A) (MRIDs 26810)  <b>Method(s):</b> 90-day feeding study in dogs</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Critical effect:</b> decreased hemoglobin and hematocrit at 4, 8, and 14 weeks) and clinical biochemistry parameters, reduced body weight gain, increased liver, spleen and kidney weights and histopathological changes in the liver.</p> <p><b>End point or Point of Departure (POD):</b> oral NOAEL = 2.5 mg/kg-day (inhalation absorption rate assumed to be 100%)</p> <p><b>Uncertainty Factors:</b> UF = 100 (10 each for intraspecies variability and interspecies extrapolation and 10x applied by MDEQ for use of subchronic study)</p> <p><b>Source and date:</b> EPA/OPP Reregistration Eligibility Decision (RED) for DCNA (Dicloran), 6/14/2006. IRIS refers to EPA-OPP for updated assessments of pesticides.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available at this time.  <b>PPRTV:</b> No PPRTV record available at this time.  <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD/AQD, no value at this time.</p>		
Inhalation Unit Risk Factor (IURF) (( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup> )	--	NA	MDEQ, 2015	
IURF details	NA	<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> CARC classified Dicloran as "Suggestive Evidence of Carcinogenic Potential"</p> <p><b>WOE Basis:</b> based on benign testicular Leydig cell tumors in male rats (1 sex, 1 species) at the high dose, which was considered adequate but not excessive, as well as a positive Ames test. In addition, there is some evidence that a plant metabolite, but not an animal metabolite, had some carcinogenic activity. No evidence of carcinogenicity was seen in mice at doses that were considered to be adequate for the assessment of carcinogenicity of dicloran.</p> <p><b>Source and Date:</b> EPA/OPP (9/5/2006) Memorandum: DICLORAN: Report of the Cancer Assessment Review Committee (CARC) PC Code: 031301 (Evaluation of the Carcinogenic Potential of Dicloran), TRX No. 0054321</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> No IRIS file available at this time. <b>PPRTV:</b> No PPRTV record available at this time. <b>MRL:</b> NA; MRLs are for non-cancer effects only.  <b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD, no value at this time.		
<b>Mutagenic Mode of Action (MMOA)? (Y/N)</b>	--	NO	USEPA, 2015	
<b>MMOA Details</b>	--	NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.		
<b>Developmental or Reproductive Effector? (Y/N)</b>	No	NO. The RfD or RfC/ITSL is not based on a reproductive-developmental effect.	MDEQ, 2015	
<b>Developmental or Reproductive Toxicity Details</b>	NA	<b>Critical Study:</b> Killeen, J. (2002) A 52-Week Oral Toxicity Study in Dogs with Dicloran: Lab Project Number: 012260-1. Unpublished study prepared by Ricerca, LLC. 329 p. (MRID 45610801) <b>Method(s):</b> One-year chronic toxicity study in dogs <b>Critical effect:</b> clinical chemistry effects (increased alkaline phosphatase in both sexes and increased cholesterol in males), increased liver weights, hepatocyte hypertrophy, vacuolar alterations of the brain and spinal cord, <b>prostate atrophy, degeneration of the seminiferous tubules, and hypospermia in the epididymides</b> <b>End point or Point of Departure (POD):</b> NOAEL = 2.5 mg/kg-day		
<b>State Drinking Water Standard (SDWS) (ug/L)</b>	--	NO	SDWA, 1976	
<b>SDWS details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
<b>Secondary Maximum Contaminant Level (SMCL) (ug/L)</b>	--	NO	SDWA, 1976 and USEPA SMCL List	

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
<b>SMCL details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List		
<b>Is there an aesthetic value for drinking water? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Aesthetic value (ug/L)</b>	NA	NA	NA	
<b>Aesthetic Value details</b>	NA	NA		
<b>Phytotoxicity Value? (Y/N)</b>	NO	Not evaluated.	NA	
<b>Phytotoxicity details</b>	NA	NA	NA	
<b>Others</b>				

**(C) Chemical-specific Exposure Factors**

	Part 201 Value	Update	Source/Reference/ Dates	Comments/Notes /Issues
Gastrointestinal absorption efficiency value (ABS <sub>gi</sub> )	---	1.0	MDEQ, 2015/USEPA RAGS-E	
ABS <sub>gi</sub> details		RAGS E (EPA, 2004) Default Value		
Skin absorption efficiency value (AE <sub>d</sub> )	---	0.1	MDEQ, 2015	
AE <sub>d</sub> details				
Ingestion Absorption Efficiency (AE <sub>i</sub> )		1.0	MDEQ, 2015	
AE <sub>i</sub> Details				
Relative Source Contribution for Water (RSC <sub>w</sub> )		0.2	MDEQ, 2015	
Relative Source Contribution for Soil (RSC <sub>s</sub> )		1.0	MDEQ, 2015	
Relative Source Contribution for Air (RSC <sub>A</sub> )		1.0	MDEQ, 2015	
Others				

**(D) Rule 57 Water Quality Values and GSI Criteria**

<b>Current GSI value (µg/L)</b>	NA
<b>Updated GSI value (µg/L)</b>	NA
<b>Rule 57 Drinking Water Value (µg/L)</b>	NA

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

Sources:

1. MDEQ Surface Water Assessment Section Rule 57 [website](#)
2. MDEQ Rule 57 [table](#)



**(E) Analytical Information**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	NA	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	0.01	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	NA	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	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