



## CHEMICAL UPDATE WORKSHEET

<b>Chemical Name:</b>	<b>n-Propyl benzene (DD)</b>
<b>CAS #:</b>	<b>103-65-1</b>
<b>Revised By:</b>	RRD Toxicology Unit
<b>Revision Date:</b>	September 24, 2015

### (A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	120.19	120.20	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	---	-99.50	EPI	EXP
Boiling Point (°C)	159.2	159.20	EPI	EXP
Solubility (ug/L)	NA	52200	EPI	EXP
Vapor Pressure (mmHg at 25°C)	NA	3.42E+00	EPI	EXP
HLC (atm-m <sup>3</sup> /mol at 25°C)	NA	1.05E-02	EPI	EXP
Log Kow (log P; octanol-water)	3.69	3.69	EPI	EXP
Koc (organic carbon; L/Kg)	4240	813.1	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm <sup>2</sup> /s)	0.08	6.02E-02	W9	EST
Diffusivity in Water (Dw; cm <sup>2</sup> /s)	8.0E-6	7.83E-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	30	CRC	EXP
Lower Explosivity Level (LEL; unitless)	NA	0.008	CRC	EXP
Critical Temperature (K)		630.00	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		9.12E+03	EPA2004	EXP
Density (g/mL, g/cm <sup>3</sup> )		0.8593	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )	NA	2.66E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )	NA	5.96E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> )	NA	4.17E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> )	NA	9.07E-05	EMSOFT	EST

**(B) Toxicity Values/Benchmarks**

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
Reference Dose (RfD) (mg/kg/day)	1.1E-2	1.0E-1	PPRTV, 2009	
RfD details	<p>Per RD: RfD is based on the RfD for isopropylbenzene. The database is insufficient to support development of an RfD for n-propylbenzene. Per Superfund Technical Support Center guidance, the RfD for isopropylbenzene (cumene) was used as a surrogate with the addition of a 10-fold uncertainty factor. CRITICAL EFFECT = increased average kidney weight. RD calculation date: 1/30/97.</p>	<p><b>Tier 2 Source:</b>  <b>PPRTV:</b>  <b>Basis:</b> PPRTV screening chronic RfD value based on EPA IRIS ethylbenzene chronic RfD surrogate.                      Per PPRTV, no chronic or subchronic p-RfD value at this time. Due to a lack of data, chronic or subchronic provisional RfDs cannot be developed. A subchronic screening p-RfD of 0.1 mg/kg/d could be developed from a 2 week ototoxicity study in rats (Gangnaire and Langlais, 2005); however, it was a single dose subchronic study and would require application of an uncertainty factor of greater than 10,000.                      PPRTV also evaluated isopropyl benzene and ethylbenzene as chemical surrogates for the development of an RfD for n-propylbenzene. Based on their analysis, PPRTV determined that ethylbenzene is the stronger surrogate candidate. The IRIS chronic RfD of 1E-01 or 0.1 mg/kg-day for ethylbenzene is recommended for the screening chronic RfD for n-propylbenzene.  <b>Source: PPRTV, 2/4/2009</b></p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available for n-propylbenzene at this time.                      Per IRIS (6/1/1991), RfD = 1.0E-1 mg/kg/day for ethylbenzene (100-41-4), a surrogate for n-propyl benzene:  <b>Critical Study:</b> Wolf, M.A., V.K. Rowe, D.D. McCollister, R.L. Hollingsworth and F. Oyen. 1956. Toxicological studies of certain alkylated benzenes and benzene. Arch. Ind. Health. 14: 387-398.  <b>Method:</b> Rat subchronic to chronic oral bioassay. The chosen study is a rat 182-day oral bioassay in which ethylbenzene was given 5 days/week at doses of 13.6, 136, 408, or 680 mg/kg/day in olive oil gavage. There were 10 albino female rats/dose group and 20 controls. The criteria considered in judging the toxic effects on the test animals were growth, mortality, appearance and behavior,</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>hematologic findings, terminal concentration of urea nitrogen in the blood, final average organ and body weights, histopathologic findings, and bone marrow counts.</p> <p><b>Critical effect:</b> Liver and kidney toxicity</p> <p><b>End point or Point of Departure (POD):</b> NOAEL 136 mg/kg/day (converted to 97.1 mg/kg/day)</p> <p><b>Uncertainty Factors:</b> UF = 1000; 10 for both interspecies and intraspecies variability to the toxicity of this chemical in lieu of specific data, and 10 for extrapolation of a subchronic effect level to its chronic equivalent</p> <p><b>Source and date:</b> IRIS (6/1/1991) for ethylbenzene (100-41-4)</p> <p><b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b>  <b>MDEQ:</b> Per DEQ-CCD/WRD (12/5/2000), RfD = 1.1E-2 mg/kg/day. A screening level was derived for n-propylbenzene using the RfD of 0.11 mg/kg/d which was derived for isopropylbenzene (cumene). An additional 10-fold uncertainty factor was applied to account for the deficiencies in the database for n-propylbenzene.</p>		
<b>Oral Cancer Slope Factor (CSF) (mg/kg-day)<sup>-1</sup></b>	NA	NA	MDEQ, 2015	
<b>CSF details</b>		<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> Per PPRTV, Inadequate information to assess the carcinogenic potential. There are no human epidemiology studies, chronic toxicity studies, or carcinogenicity assays.</p> <p><b>WOE Basis:</b> Per PPRTV, the lack of data on the carcinogenicity of n-propylbenzene precludes the derivation of quantitative estimates of risk for either oral or inhalation exposures.</p> <p><b>Source and Date:</b> PPRTV; 2/4/2009</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available for n-propyl benzene at this time.  <b>PPRTV (2/4/2990):</b> Per PPRTV, no value at this time.  <b>MRL:</b> NA; MRLs are for non-cancer effects only.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<b>Tier 3 Source:</b> <b>MDEQ:</b> Per DEQ-CCD no value at this time.		
<b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (<math>\mu\text{g}/\text{m}^3</math>)</b>	2.0E+1	1.0E+3	PPRTV, 2009	
<b>RfC/ITSL details</b>	AIR: ITSL based on rat LD <sub>50</sub> of 6040 mg/kg reported by Jenner et al (1964).	<b>Tier 2 Source:</b> <b>PPRTV:</b> <b>Basis:</b> PPRTV (2009) screening chronic RfC value based on EPA IRIS ethylbenzene chronic RfC surrogate. MDEQ (1994) is based on a LD50 value. Minnesota also adopted the PPRTV screening value. Both New York and Texas used isopropylbenzene (cumene) as chemical surrogate. <b>PPRTV (2/4/2009):</b> Per PPRTV, due to a lack of data, no chronic or subchronic RfCs are developed. PPRTV evaluated isopropyl benzene and ethylbenzene as chemical surrogates for the development of an RfC for n-propylbenzene. Based on their analysis, PPRTV determined that ethylbenzene is the stronger surrogate candidate. <ul style="list-style-type: none"> <li>Per PPRTV, inhalation values are based on using the EPA IRIS ethylbenzene RfC as a surrogate. For ethylbenzene, IRIS provides a chronic RfC of 1E+0 mg/m<sup>3</sup> (1E+3 <math>\mu\text{g}/\text{m}^3</math>) based on Andrews et al. (1981) and Hardin et al. (1981) for developmental toxicity. A chronic screening value RfC of 1E+0 mg/m<sup>3</sup> is recommended for n-propylbenzene.</li> <li>Because the IRIS RfC (for ethylbenzene) is based on developmental studies, the same value (1E+0 mg/m<sup>3</sup>) is recommended as a screening subchronic RfC. The IRIS ethylbenzene RfC is based on developmental toxicity studies (Andrew et al., 1981; Hardin et al., 1981). Subsequent developmental toxicity studies support the results of these earlier studies. The subchronic ototoxicity study by Gagnaire et al. (2007) suggests that ototoxicity may be the most sensitive endpoint for inhalation exposure to ethylbenzene. However, at this time, the best available information</li> </ul>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>supports utilization of the existing IRIS values.</p> <p><b>Tier 1 and 2 Sources:</b>  <b>IRIS:</b> No IRIS file available for n-propylbenzene at this time.  <b>Per IRIS (3/1/1991)</b>, RfC = 1E+0 mg/m<sup>3</sup> (1E+3 µg/m<sup>3</sup>) for ethylbenzene, a surrogate.  <b>Critical Study:</b> Andrew, F.D., R.L. Buschbom, W.C. Cannon, R.A. Miller, L.F. Montgomery, D.W. Phelps, et al. 1981. Teratologic assessment of ethylbenzene and 2- ethoxyethanol. Battelle Pacific Northwest Laboratory, Richland, WA. PB 83-208074, 108.  <b>Methods:</b> Inhalation experiments were conducted with Wistar rats (n=78-107/concentration) and New Zealand white rabbits (n=29-30/concentration) exposed 6 to 7 hours/day, 7 days/week during days 1-19 and 1-24 of gestation, respectively, to nominal concentrations of 0, 100, or 1000 ppm (434 or 4342 mg/cu.m) (Andrew et al., 1981). A separate group of rats was exposed pregestationally for 3 weeks prior to mating and exposure was continued into the gestational period. Actual concentrations were within 10% of target concentrations.                      All pregnant animals were sacrificed 1 day prior to term (21 days for rats; 30 days for rabbits). Maternal organs (liver, lungs, kidney, heart, spleen, adrenals, ovaries, and brain) were examined histopathologically. Uteri were examined and fetuses were weighed, sexed, and measured for crown-to-rump length, and examined for external, internal and skeletal abnormalities. For statistical analyses, the litter was chosen as the experimental unit.  <b>Critical Effect</b> Developmental toxicity  <b>End point or Point of Departure (POD):</b> NOAEL = 434 mg/m<sup>3</sup> (100 ppm)  <b>Uncertainty Factors:</b> UF = 300; 10 to protect unusually sensitive individuals, 3 to adjust for interspecies conversion and 10 to adjust for the absence of multigenerational reproductive and chronic studies  <b>Source and date:</b> IRIS; 3/1/1991 for ethylbenzene (100-41-4)   <b>MRL:</b> No MRL record available at this time.</p>		

	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p><b>Tier 3 Sources:</b>  <b>MDEQ-AQD (11/10/1994):</b> Per DEQ-CCD, ITSL = 20 mg/m<sup>3</sup>. ITSL based on rat LD<sub>50</sub> of 6,040 mg/kg reported by Jenner et al (1964).</p> <p><b>Minnesota PCA:</b> RfC= 1.00E+00 mg/m<sup>3</sup> based on PPRTV 2/7/2009.</p> <p><b>New York DEC:</b> RfC= 400 µg/m<sup>3</sup> based on based on the IRIS 2004 value for isopropylbenzene as a surrogate. A reference concentration is available for isopropylbenzene, which is structurally and chemically similar to n-propylbenzene. The similarity between the two chemicals provides a basis for using toxicity data for isopropylbenzene to represent n-propylbenzene. (Toxicity value recommendation: July, 2004)                      Source: New York State Brownfield Cleanup Program, Development of Soil Cleanup Objectives: Technical Support Document, 2006, Appendix A p2 p.A-644.</p> <p><b>Texas CEQ:</b> RfC= 4.0E-01 mg/m<sup>3</sup> (4.0E+2 µg/m<sup>3</sup>)                      Justification: N-Propylbenzene is structurally similar to Cumene, which has an IRIS RfC. Cumene is used as a surrogate for n-Propylbenzene.                      Source: TCEQ 7/22/2003 Assessment of n-Propylbenzene (In TCEQ Communication, 2015)</p> <p><b>Other Tier 3:</b> No value is available at this time from these Tier 3 sources/databases: HEAST, NTP ROC, health and environmental agencies of California, Massachusetts and New Jersey, Canada, The Netherlands (RIVM), WHO (IARC), WHO (IPCS/INCHEM), ECHA (REACH) and OECD HPV.</p>		
<b>Inhalation Unit Risk Factor (IURF) ((µg/m<sup>3</sup>)<sup>-1</sup>)</b>	NA	NA	MDEQ, 2015	
<b>IURF details</b>		<p><b>Carcinogen Weight-of-Evidence (WOE) Class:</b> Per PPRTV, Inadequate information to assess the carcinogenic potential. There are no human epidemiology studies, chronic toxicity studies, or carcinogenicity assays.</p> <p><b>WOE Basis:</b> Per PPRTV, the lack of data on the carcinogenicity of n-propylbenzene</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		precludes the derivation of quantitative estimates of risk for either oral or inhalation exposures. <b>Source and Date:</b> PPRTV; 2/4/2009  <b>Tier 1 and 2 Sources:</b> <b>IRIS:</b> No IRIS file available for n-propyl benzene at this time. <b>PPRTV (2/4/2990):</b> Per PPRTV, no value 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>	--	Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List		
<b>Developmental or Reproductive Effector? (Y/N)</b>	No	YES-inhalation the RfC is based on a reproductive-developmental effect. Inhalation Exposure Pathways- Single Exposure No-oral. The RfD is not based on a reproductive-developmental effect.	MDEQ, 2015; IRIS 3/1/1991	
<b>Developmental or Reproductive Toxicity Details</b>	NA	The RfC of the chemical surrogate, ethylbenzene, is based on a developmental effect. See RfD details above.		
<b>State Drinking Water Standard (SDWS) (µg/L)</b>	NO	NO	SDWA, 1976	
<b>SDWS details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
<b>Secondary Maximum Contaminant Level (SMCL) (µg/L)</b>	NO	NO	SDWA, 1976 and USEPA SMCL List	
<b>SMCL details</b>	NA	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		

	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
Is there an Aesthetic Value? (Y/N)	NO	Not evaluated.	NA	
Aesthetic value details	NA	NA		
Is there a Phytotoxicity Value? (Y/N)	NO	Not evaluated.	NA	
Phytotoxicity details	NA	NA		
Others:				

**(C) Chemical-specific Absorption 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, 2004	
ABS <sub>gi</sub> details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (A <sub>Ed</sub> )	---	0.1	MDEQ, 2015	
A <sub>Ed</sub> details				
Ingestion Absorption Efficiency (A <sub>Ei</sub> )		1.0	MDEQ, 2015	
A <sub>Ei</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>	ID
<b>Updated GSI value (µg/L)</b>	ID
<b>Rule 57 Drinking Water Value (µg/L)</b>	ID

	<b>Rule 57 Value (µg/L)</b>	<b>Verification Date</b>
<b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>	ID	11/2000
<b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b>	ID	11/2000
<b>Wildlife Value (WV)</b>	NA	NA
<b>Human Cancer Values for Drinking Water Source (HCV-drink)</b>	NA	NA
<b>Human Cancer values for non-drinking water source (HCV-Non-drink)</b>	NA	NA
<b>Final Chronic Value (FCV)</b>	ID	9/2006
<b>Aquatic maximum value (AMV)</b>	ID	9/2006
<b>Final Acute Value (FAV)</b>	ID	9/2006

Sources:

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



**(E) Target Detection Limits (TDL)**

	<b>Value</b>	<b>Source</b>
<b>Target Detection Limit – Soil (<math>\mu\text{g}/\text{kg}</math>)</b>	100	MDEQ, 2015
<b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b>	1	MDEQ, 2015
<b>Target Detection Limit – Air (ppbv)</b>	4.00E+00	MDEQ, 2015
<b>Target Detection Limit – Soil Gas (ppbv)</b>	1.30E+02	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 OEHHHA	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

