



CHEMICAL UPDATE WORKSHEET

Chemical Name:	Isopropyl benzene (Cumene)
CAS #:	98-82-8
Revised By:	RRD Toxicology Unit
Revision Date:	September 24, 2015

(A) Chemical-Physical Properties

	Part 201 Value	Updated Value	Reference Source	Comments
Molecular Weight (g/mol)	122.16	120.20	EPI	EXP
Physical State at ambient temp	Liquid	Liquid	MDEQ	
Melting Point (°C)	177	-96.00	EPI	EXP
Boiling Point (°C)	152.4	152.40	EPI	EXP
Solubility (ug/L)	56000	61300	EPI	EXP
Vapor Pressure (mmHg at 25°C)	0.006	4.50E+00	EPI	EXP
HLC (atm-m³/mol at 25°C)	1.50E-2	1.15E-02	EPI	EXP
Log Kow (log P; octanol-water)	3.6	3.66	EPI	EXP
Koc (organic carbon; L/Kg)	3460	697.8	EPI	EST
Ionizing Koc (L/kg)		NR	NA	NA
Diffusivity in Air (Di; cm²/s)	0.086	6.03E-02	W9	EST
Diffusivity in Water (Dw; cm²/s)	7.1E-6	7.86E-06	W9	EST
Soil Water Partition Coefficient (Kd; inorganics)	NR	NR	NA	NA

	Part 201 Value	Updated Value	Reference Source	Comments
Flash Point (°C)	96 F	36	CRC	EXP
Lower Explosivity Level (LEL; unitless)	0.009	0.009	CRC	EXP
Critical Temperature (K)		631.10	EPA2004	EXP
Enthalpy of Vaporization (cal/mol)		1.03E+04	EPA2004	EXP
Density (g/mL, g/cm ³)		0.864	CRC	EXP
EMSOFT Flux Residential 2 m (mg/day/cm ²)	2.27E-05	2.68E-05	EMSOFT	EST
EMSOFT Flux Residential 5 m (mg/day/cm ²)	4.15E-05	6.08E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 2 m (mg/day/cm ²)	3.12E-05	4.21E-05	EMSOFT	EST
EMSOFT Flux Nonresidential 5 m (mg/day/cm ²)	5.35E-05	9.32E-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-1	1.0E-1	IRIS, 1997	
RfD details	Rat gavage subchronic study (Wolf et al., 1956); NOAEL = 110 mg/kg-day; UF=1000; Critical effect = increased average kidney weight. An additional UF of 3 was applied by EPA to account for inadequate reproductive tox data -- this was not applied consistent with DEQ policy.	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. IRIS RfD = 1.0E-1 mg/kg/day Critical Study: 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. Method: Groups of 10 female Wistar rats were administered 139 doses of cumene by gavage in olive oil at 154, 462, or 769 mg/kg-day over a 194-day period; 20 rats given olive oil served as controls. Critical effect: Increased average kidney weight in female rats. End point or Point of Departure (POD): NOAEL: 154 mg/kg-day adjusted to 110 mg/kg-day based on the dosing schedule. LOAEL: 462 mg/kg-day adjusted to 331 mg/kg-day based on the dosing schedule. Uncertainty Factors: UF = 1,000 (10 for intraspecies variability, 10 for interspecies extrapolation, 3 for subchronic-to-chronic duration extrapolation, and 3 for database deficiencies (lack of reproductive information). Justification for the use of a partial UF for subchronic-to-chronic extrapolation was that the duration of the study (6 to 7 months) is intermediate between subchronic (3 months) and chronic (24 months) duration. Source and date: IRIS, 08/01/1997</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/RRD: Per DEQ-CCD, RfD = 0.11 mg/kg/d. Wolf et al., 1956.</p>		Complete
Oral Cancer Slope Factor (CSF)	NA	NA	MDEQ, 2015	



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
(mg/kg-day) ⁻¹)				
CSF details		<p>IRIS carcinogenicity weight of evidence Characterization: Classification – D; not classifiable as to human carcinogenicity. IRIS 8/1/1997</p> <p>Tier 1 and 2 Sources: IRIS: IRIS (1997) indicates that CSF is not available PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Source: MDEQ/RRD: Per DEQ-CCD, no value.</p>		Complete
Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³)	8.7E+1	4.0E+2	IRIS, 1997	
RfC/ITSL details	Per AQD: ITSL based on NOAEL of 100 ppm from Union Carbide (1991) 13 week inhalation study in rats.	<p>Tier 1 Source: IRIS: Basis: IRIS is a Tier 1 source. IRIS RfC = 4.0E+2 µg/m³.</p> <p>Critical Study: Cushman, J.R., J.C. Norris, D.E. Dodd, K.I. Darmer, and C.R. Morris. (1995) Subchronic inhalation toxicity and neurotoxicity assessment of cumene in Fischer 344 rats. J. Am. Coll. Toxicol. 14(2): 129-147.</p> <p>Method: Two successive subchronic inhalation toxicity studies with cumene vapor (>99.9% pure) were conducted on Fischer 344 rats. In the first study, groups, (21/sex) were exposed to 0, 100, 496, or 1,202 ppm (0, 492, 2,438, or 5,909 mg/m³, respectively) cumene vapor for 6 hours/day, 5 days/week, for 13 weeks (duration adjusted to 0, 88, 435, and 1055 mg/m³). In the second study, the group size was decreased to 15/sex, an additional group (50 ppm, duration adjusted to 44 mg/m³) was added, and a 4-week post-exposure recovery period was incorporated at the end of the experiment.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/Date	Comments/Notes/Issues
		<p>Critical effect: Increased relative and absolute kidney weights in female rats and relative and absolute adrenal weights in male and female rats.</p> <p>End point or Point of Departure (POD): NOAEL: 2,438 mg/m³ (496 ppm); NOAEL_{ADJ} & NOAEL_{HEC}: 435 mg/m³; LOAEL: 5,909 mg/m³ (1202 ppm); LOAEL_{ADJ} & LOAEL_{HEC}: 1,055 mg/m³. Conversion factors and assumption: MW = 120.2. assuming 25°C and 760 mmHg, NOAEL (mg/m³) = 496 ppm x 120.2/24.45 = 2,438 mg/m³. NOAEL_{ADJ} = NOAEL (mg/m³) x 6 hours/24 hours x 5/7 days = 435 mg/m³. The NOAEL_{HEC} was calculated for a gas:extrarrespiratory (systemic) effect assuming periodicity was obtained. Because the b:a lambda values are unknown for the experimental animal species and humans, a default value of 1 is used for this ratio. NOAEL_{HEC} = NOAEL_{ADJ} x b:a lambda(a) / b:a lambda(h) = 435 mg/m³.</p> <p>Uncertainty Factors: UF = 1,000. (10 for subchronic-to-chronic extrapolation, 10 for intraspecies variability, 3 for interspecies extrapolation, and 3 for database deficiencies (lack of reproductive studies)).</p> <p>Source and date: IRIS, 08/01/1997.</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/AQD: Per DEQ-CCD, ITSL = 400 ug/m³; 24 hr. averaging time; ITSL is based on the EPA 1997 RfC of 400 ug/m³. This RfC is based on the Cushman et al (1995) NOAEL for increased kidney weight and adrenal weights at a dose of 496 ppm in a rat 13 week inhalation study as described above.</p>		
Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹)	NA	1.05E-5	MDEQ, 2010	
IURF details		<p>Tier 3 Source: MDEQ: Basis: MDEQ value based on a chronic inhalation toxicity study (NTP, 2009). No value is available from other Tier 3 sources. See details below.</p>		Complete



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		<p>Tier 1 and 2 Sources: IRIS: The IRIS file is dated 08/01/1997, which predates the NTP (2009) study described below. IRIS indicates that data and an IUR are not available. PPRTV: No PPRTV record available at this time. MRL: NA; MRLs are for non-cancer effects only.</p> <p>Tier 3 Sources: MDEQ-AQD 02/25/2010: IURF = 1.05E-5 per µg/m³. Critical Study: NTP, 2009. Toxicology and carcinogenesis studies of cumene in F344 rat and B6C3F1 mice. NTP TR-542. Method: 50 individual female and male F344/N rats and B6C3F1 mice were placed in groups and exposed to varied concentrations of cumene. Male and female rats and male mice were exposed to 250, 500, or 1,000 ppm cumene with a chamber control group. Female mice were exposed to 125, 250, or 500 ppm cumene with a chamber control group. Each group was exposed in an inhalation chamber for 6 hours/day, 5 days/week for 105 weeks. WOE Basis: The NTP (2009) report concluded that there was a clear evidence of carcinogenic activity in male rats due to a statistically significant increase in respiratory epithelial adenoma in the nose (0/40, 7/38, 18/42, 10/44) and renal tubule adenomas or carcinomas combined (2/40, 5/38, 8/42, 7/44). There was some evidence of carcinogenic activity in female rats due to an increased incidence of respiratory epithelium adenoma in the nose (0/26, 5/28, 4/32, 3/32). There was also clear evidence of carcinogenic activity in male and female mice based on a statistically significant increase in incidences of alveolar/bronchiolar neoplasms (male mice: 19/50, 38/50, 42/49, 43/47 and female mice 4/47, 31/49, 32/50, 46/50). Source and Date: MDEQ, 02/25/2010.</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 California, Massachusetts, Minnesota, New Jersey, New York, and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and</p>		



	Part 201 Value	Updated Value	Source/Reference/ Date	Comments/Notes /Issues
		OECD HPV.		
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, the RfD and the RfC are not based on a reproductive-developmental effect.	MDEQ, 2015	
Developmental or Reproductive Toxicity Details	--			
State Drinking Water Standard (SDWS) (µg/L)	--	NO	SDWA, 1976	
SDWS details	--	MI Safe Drinking Water Act (SDWA) 1976 PA 399		
Secondary Maximum Contaminant Level (SMCL) (µg/L)	--	NO	SDWA, 1976 and USEPA SMCL List	
SMCL details	--	MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015		
Is there an Aesthetic Value? (Y/N)	NA	Not evaluated.	NA	
Aesthetic value details	NA	NA		
Is there a Phytotoxicity Value? (Y/N)	NA	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 _{gi})	---	1.0	MDEQ, 2015/USEPA RAGS-E, 2004	
ABS _{gi} details		RAGS E (USEPA, 2004) Default Value		
Skin absorption efficiency value (A _{Ed})	---	0.1	MDEQ, 2015	
A _{Ed} details				
Ingestion Absorption Efficiency (A _{Ei})		1.0	MDEQ, 2015	
A _{Ei} 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)	28
Updated GSI value (µg/L)	28
Rule 57 Drinking Water Value (µg/L)	1,700

	Rule 57 Value (µg/L)	Verification Date
Human Non-cancer Values- Drinking water source (HNV-drink)	1,700	3/2011
Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)	3,800	3/2011
Wildlife Value (WV)	NA	
Human Cancer Values for Drinking Water Source (HCV-drink)	NA	
Human Cancer values for non-drinking water source (HCV-Non-drink)	NA	
Final Chronic Value (FCV)	28	7/2008
Aquatic maximum value (AMV)	250	7/2008
Final Acute Value (FAV)	500	7/2008

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 ($\mu\text{g}/\text{kg}$)	250	MDEQ, 2015
Target Detection Limit – Water ($\mu\text{g}/\text{L}$)	5	MDEQ, 2015
Target Detection Limit – Air (ppbv)	4.90E-01	MDEQ, 2015
Target Detection Limit – Soil Gas (ppbv)	1.60E+01	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