



CHEMICAL UPDATE WORKSHEET

| | |
|-----------------------|-------------------------|
| Chemical Name: | Diisopropylamine |
| CAS #: | 108-18-9 |
| 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) | 101.22 | 101.19 | EPI | EXP |
| Physical State at ambient temp | Liquid | Liquid | MDEQ | |
| Melting Point (°C) | --- | -61.00 | EPI | EXP |
| Boiling Point (°C) | 83.57 | 83.90 | EPI | EXP |
| Solubility (ug/L) | 3.69E+7 | 1.1E+08 | EPI | EXP |
| Vapor Pressure (mmHg at 25°C) | 74.552 | 7.94E+01 | EPI | EXP |
| HLC (atm-m ³ /mol at 25°C) | 9.60E-5 | 9.60E-05 | PP | EST |
| Log Kow (log P; octanol-water) | 1.6 | 1.40 | EPI | EXP |
| Koc (organic carbon; L/Kg) | 37.4 | 63.66 | EPI | EST |
| Ionizing Koc (L/kg) | | NR | NA | NA |
| Diffusivity in Air (Di; cm ² /s) | 0.08 | 6.59E-02 | W9 | EST |
| Diffusivity in Water (Dw; cm ² /s) | 8.0E-6 | 7.7783E-06 | W9 | EST |
| Soil Water Partition Coefficient (Kd; inorganics) | NR | NR | NA | NA |

| | Part 201 Value | Updated Value | Reference Source | Comments |
|--|----------------|---------------|------------------|----------|
| Flash Point (°C) | 20 F | -1 | CRC | EXP |
| Lower Explosivity Level (LEL; unit less) | 0.011 | 0.011 | CRC | EXP |
| Critical Temperature (K) | | 523.1 | CRC | EXP |
| Enthalpy of Vaporization (cal/mol) | | 7.27E+03 | CRC | EXP |
| Density (g/mL, g/cm ³) | | 0.7153 | CRC | EXP |
| EMSOFT Flux Residential 2 m (mg/day/cm ²) | 2.04E-05 | 2.28E-05 | EMSOFT | EST |
| EMSOFT Flux Residential 5 m (mg/day/cm ²) | 3.13E-05 | 3.94E-05 | EMSOFT | EST |
| EMSOFT Flux Nonresidential 2 m (mg/day/cm ²) | 2.74E-05 | 3.43E-05 | EMSOFT | EST |
| EMSOFT Flux Nonresidential 5 m (mg/day/cm ²) | 3.86E-05 | 5.37E-05 | EMSOFT | EST |

(B) Toxicity Values/Benchmarks

| | Part 201 Value | Updated Value | Source/Reference/Date | Comments/Notes/Issues |
|----------------------------------|--|---|-----------------------|-----------------------|
| Reference Dose (RfD) (mg/kg/day) | 7.7E-4 | 7.7E-4 | MDEQ, 1994 | |
| RfD details | Oral male Wistar rat LD 50 of 770mg/kg (Smyth 1954) (UF = 100, acute-to-chronic application factor = 0.0001). CCD/RRD date: 1/5/1994. | <p>Tier 3 Source: MDEQ: Basis: MDEQ derived a RfD = 1.7E-2 mg/kg-day value using the NOAEL of 15 mg/kg-day from the subacute study in ECHA and a total UF of 3000 (10 each for interspecies extrapolation, interspecies variability, and subacute to chronic exposure and 3 for database deficiency). The ECHA UF used a 6 for subacute to chronic extrapolation and did not include database deficiency considerations.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: Critical Study: Smyth HF Jr, Carpenter CP, Weil CS, Pozzani UC (1954). Range-finding toxicity data: list V. AMA Arch Ind Hyg Occup Med 10:61-68. Method(s): male Wistar rats were exposed orally; 4-hour exposure to 1,000 ppm killed 2 of 6 rats Critical effect: death End point or Point of Departure (POD): rat LD 50 = 770mg/kg Uncertainty Factors: UF = 100 and acute-to-chronic application factor = 0.0001 Source and date: MDEQ-CCD/RRD, 1/05/1994</p> <p>ECHA: Derived No Effect Level (DNEL) = 83 µg/kg bw/day. DNEL basis: Key study: Study report, 1991 Guideline: EU Method B.7 (Repeated Dose (28 Days) Toxicity (Oral)) Method: Subacute study; male and female Sprague Dawley rats were exposed to 0, 15, 50, and 150 mg/kg/day diisopropylamine by gavage (oral) daily for 4 weeks.</p> | | Complete |



| | Part 201 Value | Updated Value | Source/Reference/Date | Comments/Notes/Issues |
|--|----------------|---|-----------------------|-----------------------|
| | | <p>Critical effect: mortality, body weight, haematological and clinical chemistry changes Dose descriptor starting point: NOAEL - 50 mg/kg/day NOAEL – 15 mg/kg-day for gastric irritation Overall assessment factor (AF): 600 AF for differences in duration of exposure: 6 AF for interspecies differences (allometric scaling): 4 AF for other interspecies differences: 2.5 AF for interspecies differences: 10 Source: ECHA REACH Dossier on Diisopropylamine</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), and OECD HPV.</p> | | |
| Oral Cancer Slope Factor (CSF) (mg/kg-day)⁻¹ | -- | NA | MDEQ, 2015 | |
| CSF details | NA | <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. 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 (RfC) or Initial Threshold Screening Level (ITSL) (µg/m³) | -- | 2.0E+2 | MDEQ, 1998 | |
| RfC/ITSL details | NA | <p>Tier 3 Source: MDEQ:</p> | | Complete |



| | Part 201 Value | Updated Value | Source/Reference/ Date | Comments/Notes /Issues |
|--|----------------|---|---------------------------|---------------------------|
| | | <p>Basis: MDEQ value based on a NIOSH REL which used an 8-week inhalation study of four animal species. The ECHA value is based on a 4-week rat study. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: No PPRTV record available at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 sources: MDEQ: AQD (1998) ITSL = 2.0E+2 µg/m³: ITSL is based on NIOSH REL of 20 mg/m³ TWA. Averaging time = 8 hours. Justification: In a sub chronic inhalation study by Treon et al. (1949), groups of guinea pigs, rabbits, cats, and rats were exposed 7 hr. /day over an eight week period. All rabbits died by the 20th exposure day, as well as one-half of the guinea pigs, but all other test animals survived the 40 exposures at 600 ppm. No changes were seen in the cellular elements of the blood in any of the exposed animals; however, cloudiness of the cornea with partial or total loss of vision occurred. Treon also cited reports of disturbances in vision, nausea, and headache in workers at levels between 25 and 50 ppm. Based upon limited data, the ACGIH recommended a threshold limit value (TLV) of 5 ppm (21 mg/m³) to protect against disturbance of vision and irritation of respiratory passages. NIOSH confirmed this value by also establishing a recommended exposure level (REL) of 5 ppm, but because of rounding differences, converted the REL to 20 mg/m³. ITSL Calculation: ITSL = REL / 100 = 0.2 mg/m³ Source and date: MDEQ-CCD/AQD, 8/20/1998.</p> <p>ECHA: RfC=0.6 mg/m³ based on? DNEL (Derived No Effect Level) basis: Key study: Val Roloff, 1987 Guideline: EU Method B.7 (Repeated Dose (28 Days) Toxicity (Oral)) Method: Subacute study; Sprague-Dawley rats (15/sex/concentration) were</p> | | |



| | Part 201 Value | Updated Value | Source/Reference/ Date | Comments/Notes /Issues |
|--|----------------|---|---------------------------|---------------------------|
| | | <p>administered DIPA as a vapor at 0, 0.1, 0.6 and 2 mg/L (100, 620 and 2000 mg/m³) via whole body inhalation for 6 hours per day, 5 days per week for approximately one month (maximum of 23 exposures).</p> <p>Critical effect: decreased body weight and changes in blood parameters; lymphocytopenia in males and lesions in the cornea and nasal passages</p> <p>Dose descriptor starting point: LOAEC - 100 mg/m³ (0.1 mg/L)</p> <p>NOAEL – 15 mg/kg-day for gastric irritation</p> <p>Calculation – not specified</p> <p>Source: ECHA REACH Dossier on Diisopropylamine</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), and OECD HPV.</p> | | |
| Inhalation Unit Risk Factor (IURF) (($\mu\text{g}/\text{m}^3$) ⁻¹) | -- | NA | MDEQ, 2015 | |
| IURF details | NA | <p>Tier 1 and 2 Sources:</p> <p>IRIS: No IRIS file available at this time.</p> <p>PPRTV: No PPRTV record available at this time.</p> <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> | | Complete |
| Mutagenic Mode of Action (MMOA)? (Y/N) | -- | NO | USEPA, 2015 | |
| MMOA Details | -- | <p>NA</p> <p>Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List.</p> | | |
| Developmental or Reproductive Effector? (Y/N) | No | No. The RfD or RfC/ITSL is not based on a reproductive-developmental effect. | MDEQ, 2015 | |

| | Part 201 Value | Updated Value | Source/Reference/ Date | Comments/Notes /Issues |
|--|----------------|---|--------------------------------------|---------------------------|
| Developmental or Reproductive Toxicity Details | NA | NA | | |
| State Drinking Water Standard (SDWS) (ug/L) | -- | NO | 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, 2015 | |
| SMCL details | NA | SDWA, 1976 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 | |
| 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) | NA |
| Updated GSI value (µg/L) | NA |
| Rule 57 Drinking Water Value (µg/L) | NA |

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

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 ($\mu\text{g}/\text{L}$) | NA | MDEQ, 2015 |
| Target Detection Limit – Air (ppbv) | 4.80E+01 | MDEQ, 2015 |
| Target Detection Limit – Soil Gas (ppbv) | 1.60E+03 | 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 |