



## CHEMICAL UPDATE WORKSHEET

|                       |                     |
|-----------------------|---------------------|
| <b>Chemical Name:</b> | <b>Acetone</b>      |
| <b>CAS #:</b>         | <b>67-64-1</b>      |
| <b>Revised By:</b>    | RRD Toxicology Unit |
| <b>Revision Date:</b> | November 14, 2015   |

### (A) Chemical-Physical Properties

|  | Part 201 Value | Updated Value | Reference Source | Comments |
|--|----------------|---------------|------------------|----------|
| <b>Molecular Weight (g/mol)</b>                          | 58.08          | 58.08         | EPI              | EXP      |
| <b>Physical State at ambient temp</b>                    | Liquid         | Liquid        | MDEQ             |          |
| <b>Melting Point (°C)</b>                                | 179            | -94.8         | EPI              | EXP      |
| <b>Boiling Point (°C)</b>                                | 56             | 56.00         | EPI              | EXP      |
| <b>Solubility (ug/L)</b>                                 | 1.0E+9         | 1.00E+09      | EPI              | EXP      |
| <b>Vapor Pressure (mmHg at 25°C)</b>                     | 228            | 2.32E+02      | EPI              | EXP      |
| <b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>               | 3.88E-5        | 3.50E-05      | EPI              | EXP      |
| <b>Log Kow (log P; octanol-water)</b>                    | -0.240         | -0.24         | EPI              | EXP      |
| <b>Koc (organic carbon; L/Kg)</b>                        | 0.581          | 2.364         | EPI              | EST      |
| <b>Ionizing Koc (L/kg)</b>                               |                | NR            | NA               | NA       |
| <b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>         | 0.124          | 1.06E-01      | W9               | EST      |
| <b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>       | 1.14E-5        | 1.1471E-05    | W9               | EST      |
| <b>Soil Water Partition Coefficient (Kd; inorganics)</b> | NR             | NR            | NA               | NA       |

|  | Part 201 Value | Updated Value | Reference Source | Comments |
|--|----------------|---------------|------------------|----------|
| Flash Point (°C)   | 0.0 F          | -20           | CRC              | EXP      |
| Lower Explosivity Level (LEL; unit less)                 | 0.025          | 0.025         | CRC              | EXP      |
| Critical Temperature (K)                                 |                | 508.10        | EPA2001          | EXP      |
| Enthalpy of Vaporization (cal/mol)                       |                | 6.96E+03      | EPA2001          | EXP      |
| Density (g/mL, g/cm <sup>3</sup> )                       |                | 0.7845        | CRC              | EXP      |
| EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )    | 2.28E-05       | 2.48E-05      | EMSOFT           | EST      |
| EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )    | 4.19E-05       | 4.96E-05      | EMSOFT           | EST      |
| EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> ) | 3.14E-05       | 4.96E-05      | EMSOFT           | EST      |
| EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> ) | 5.41E-05       | 7.17E-05      | EMSOFT           | EST      |

**(B) Toxicity Values/Benchmarks**

|  | Part 201 Value  | Updated Value  | Source/Reference/Date | Comments/Notes/Issues |
|--|---|--|-----------------------|-----------------------|
| Reference Dose (RfD) (mg/kg/day)                         | 1.0E-1  | 9.0E-1   | IRIS, 2003            |                       |
| RfD details  | Subchronic (gavage) oral rat study (90 days), NOAEL = 100 mg/kg/day<br>Critical effect = increased liver & kidney weights & nephrotoxicity (US EPA, 1986) | <p><b>Tier 1 Source:</b><br/> <b>IRIS:</b><br/> <b>Basis:</b> IRIS is a Tier 1 Source.<br/> <b>Critical Studies:</b> (Dietz et al., 1991; NTP, 1991).<br/>                     1) Dietz, DD; Leininger, JR; Rauckman, EJ; et al. (1991) Toxicity studies of acetone administered in the drinking water of rodents. Fund. Appl. Toxicol. 17:347-360.<br/>                     2) NTP (National Toxicology Program). (1991) Toxicity studies of acetone (CAS No. 67-64-1) in F344/N rats and B6C3F1 mice (drinking water studies). NTP, Research Triangle Park, NC. NTP TOX 3, NIH Publication No. 91-3122.<br/> <b>Method(s):</b> subchronic drinking water study; F344/N rats (n=10/dose/sex); 0, 2,500, 5,000, 10,000, 20,000, or 50,000 ppm for 13 weeks<br/> <b>Critical effect:</b> testicular, renal and hematology changes in male rats.<br/> <b>End point or Point of Departure (POD):</b> NOAEL = 900 mg/kg-day<br/> <b>Uncertainty Factors:</b> UF = 1,000 (10 each for intraspecies variability and database deficiency and 3 each for interspecies and subchronic to chronic extrapolation)<br/> <b>Source and date:</b> IRIS; Last revision date - 07/31/2003</p> <p><b>Tier 2 Sources:</b><br/> <b>PPRTV:</b> No PPRTV record available at this time.<br/> <b>MRL:</b> Per ATSDR (05/1994), no chronic oral MRL at this time. Intermediate oral MRL = 2 mg/kg/day is based on hematological effect and UF = 100. From 12/2014 ATSDR MRL list.</p> <p><b>Tier 3 Source:</b><br/> <b>MDEQ:</b> Per CCD/RRD, RfD = 1.0E-1 mg/kg-day. See Part 201 Value RfD details.</p> |                       | Complete              |
| Oral Cancer Slope Factor (CSF) (mg/kg-day) <sup>-1</sup> | --  | NA   | MDEQ, 2015            |                       |
| CSF details  | NA  | <b>Carcinogen Weight-of-Evidence (WOE) Class:</b> data are inadequate for an assessment of the human carcinogenic potential of acetone   |                       | Complete              |



|  | Part 201 Value  | Updated Value   | Source/Reference/Date | Comments/Notes/Issues |
|--|---|---|-----------------------|-----------------------|
|  |   | <p><b>IRIS WOE Basis:</b> based on the availability of one human study of limited utility, no chronic animal studies, and no additional information on structural analogues with known carcinogenic potential. Acetone has tested negative in almost all genotoxicity studies.<br/> <b>Source and Date:</b> IRIS, Last revision date - 7/31/2003.</p> <p><b>Tier 1 and 2 Sources:</b><br/> <b>IRIS:</b> Per IRIS (7/31/2003), no value at this time.<br/> <b>PPRTV:</b> No PPRTV record available at this time.<br/> <b>MRL:</b> NA; ATSDR MRLs are for non-cancer health effects only.</p> <p><b>Tier 3 Source:</b><br/> <b>MDEQ:</b> Per CCD/RRD, no value at this time.</p>  |                       |                       |
| <b>Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) (<math>\mu\text{g}/\text{m}^3</math>)</b> | 5.9E+3  | 3.1E+4  | ATSDR, 1994           |                       |
| <b>RfC/ITSL details</b>  | ITSL based on 1985 NIOSH REL, 250 ppm or 590 mg/m <sup>3</sup> . Inhalation data is insufficient to calculate an RfC. It is inappropriate to convert RfD to air value based on comparison of NOAEL mg/kg dose.<br>CCD-AQD date: | <p><b>Tier 2 Source:</b><br/> <b>ATSDR:</b><br/> <b>Basis:</b> ATSDR is a Tier 2 source, Tier 1 not available.<br/>                     Chronic MRL = 13 ppm or 30.9 mg/ m<sup>3</sup> (3.1E+4 <math>\mu\text{g}/\text{m}^3</math>); (13ppm*58.08g/mol) /24.45L (SATP) = 30.9 mg/m<sup>3</sup>.<br/> <b>Critical Study:</b> Stewart, RD; Hake, CL; Wu, A; et al. (1975) Acetone: development of a biologic standard for the industrial worker by breath analysis. Medical College of Wisconsin, Inc., Milwaukee. Dept. of Environmental Medicine. U.S Dept. of Commerce. NTIS PB82172917. (Stewart et al. 1975)<br/> <b>Method(s):</b> human volunteers were exposed to acetone &lt;1,250 ppm for &lt;7.5 hours/day for 6 weeks<br/> <b>Critical effect:</b> neurological effects (increased visual evoked response)<br/> <b>End point or Point of Departure (POD):</b> LOAEL = 1,250 ppm<br/> <b>Uncertainty Factors:</b> UF = 100; 10-fold for use as a LOAEL and 10-fold for human</p> |                       | Complete              |



|   | Part 201 Value  | Updated Value   | Source/Reference/<br>Date | Comments/Notes<br>/Issues |
|---|---|---|---------------------------|---------------------------|
|   | 6/18/92<br><br>Using Rule 232(1)<br>(c) for calculating<br>an ITSL based on<br>an occupational<br>exposure level<br>(OEL), ITSL = 590<br>mg/m <sup>3</sup> ÷ 100 =<br>5.9 mg/m <sup>3</sup> or<br>5,900 ug/m <sup>3</sup> . | variability<br><b>Source and date:</b> ATSDR, 5/1994<br><br><b>Tier 1 and 2 Sources:</b><br><b>IRIS:</b> Per IRIS, no value at this time.<br><b>PPRTV:</b> No PPRTV record available at this time.<br><br><b>Tier 3 source:</b><br><b>MDEQ:</b> Per DEQ-CCD/AQD (6/18/1992), ITSL = 5.9E+3 µg/m <sup>3</sup> . See Part 201 Value<br>RfC/ITSL details.  |                           |                           |
| <b>Inhalation Unit<br/>Risk Factor<br/>(IURF) ((µg/m<sup>3</sup>)<sup>-1</sup>)</b> | --  | NA  | MDEQ, 2015                |                           |
| <b>IURF details</b>   | NA  | <b>Carcinogen Weight-of-Evidence (WOE) Class:</b> data are inadequate for an<br>assessment of the human carcinogenic potential of acetone<br><b>IRIS WOE Basis:</b> based on the availability of one human study of limited utility, no<br>chronic animal studies, and no additional information on structural analogues<br>with known carcinogenic potential. Acetone has tested negative in almost all<br>genotoxicity studies.<br><b>Source and Date:</b> IRIS, Last revision date - 7/31/2003.<br><br><b>Tier 1 and 2 Sources:</b><br><b>IRIS:</b> Per IRIS (7/31/2003), no value at this time.<br><b>PPRTV:</b> No PPRTV record available at this time.<br><b>MRL:</b> NA; ATSDR MRLs are for non-cancer health effects only.<br><br><b>Tier 3 Source:</b><br><b>MDEQ:</b> Per CCD/RRD, no value at this time. |                           | Complete                  |
| <b>Mutagenic Mode<br/>of Action<br/>(MMAO)? (Y/N)</b>                               | --  | NO  | USEPA, 2015               |                           |

|  | Part 201 Value | Updated Value  | Source/Reference/<br>Date       | Comments/Notes<br>/Issues |
|--|----------------|--|---------------------------------|---------------------------|
| <b>MMOA Details</b>  | --             | NA<br>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 ITSL is not based on a reproductive-developmental effect.     | MDEQ, 2015                      |                           |
| <b>Developmental or Reproductive Toxicity Details</b>        | NA             | NA   |                                 |                           |
| <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 Lists |                           |
| <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             | NO   | NA                              |                           |
| <b>Is there an Aesthetic value (ug/L)</b>                    | NA             | Not evaluated.   | 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/<br>Dates | Comments/Notes<br>/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>            | 1,700 |
| <b>Updated GSI value (µg/L)</b>            | 1,700 |
| <b>Rule 57 Drinking Water Value (µg/L)</b> | 5,600 |

|  | <b>Rule 57 Value<br/>(µg/L)</b> | <b>Verification Date</b> |
|--|---------------------------------|--------------------------|
| <b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>          | 5,600                           | 10/1997                  |
| <b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b> | 450,000                         | 10/1997                  |
| <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>   | 1,700                           | 11/1997                  |
| <b>Aquatic maximum value (AMV)</b>   | 15,000                          | 11/1997                  |
| <b>Final Acute Value (FAV)</b>   | 30,000                          | 11/1997                  |

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> | 1,000        | MDEQ, 2015    |
| <b>Target Detection Limit – Water (<math>\mu\text{g}/\text{L}</math>)</b> | 50           | MDEQ, 2015    |
| <b>Target Detection Limit – Air (ppbv)</b>                                | 2.50E+03     | MDEQ, 2015    |
| <b>Target Detection Limit – Soil Gas (ppbv)</b>                           | 8.20E+04     | 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     |