



## CHEMICAL UPDATE WORKSHEET

|                       |                     |
|-----------------------|---------------------|
| <b>Chemical Name:</b> | <b>Nitrate (DD)</b> |
| <b>CAS #:</b>         | <b>14797-55-8</b>   |
| <b>Revised By:</b>    | RRD Toxicology Unit |
| <b>Revision Date:</b> | August 18, 2015     |

### (A) Chemical-Physical Properties

|  | Part 201 Value | Updated Value | Reference Source | Comments |
|--|----------------|---------------|------------------|----------|
| <b>Molecular Weight (g/mol)</b>                          | 62             | 62.00         | EPI              | EXP      |
| <b>Physical State at ambient temp</b>                    | Inorganic      | Inorganic     | MDEQ             |          |
| <b>Melting Point (°C)</b>                                | ---            | NA            | NA               |          |
| <b>Boiling Point (°C)</b>                                | ---            | NA            | NA               |          |
| <b>Solubility (ug/L)</b>                                 | NA             | NA            | NA               | NA       |
| <b>Vapor Pressure (mmHg at 25°C)</b>                     | NA             | NR            | NA               | NA       |
| <b>HLC (atm-m<sup>3</sup>/mol at 25°C)</b>               | NR             | NR            | NA               | NA       |
| <b>Log Kow (log P; octanol-water)</b>                    | NR             | NR            | NA               | NA       |
| <b>Koc (organic carbon; L/Kg)</b>                        | NR             | NR            | NA               | NA       |
| <b>Ionizing Koc (L/kg)</b>                               |                | NR            | NA               | NA       |
| <b>Diffusivity in Air (Di; cm<sup>2</sup>/s)</b>         | NR             | NR            | NA               | NA       |
| <b>Diffusivity in Water (Dw; cm<sup>2</sup>/s)</b>       | NR             | NR            | NA               | NA       |
| <b>Soil Water Partition Coefficient (Kd; inorganics)</b> | NA             | NA            | NA               | NA       |

|  | Part 201 Value | Updated Value | Reference Source | Comments |
|--|----------------|---------------|------------------|----------|
| Flash Point (°C)   | NA             | NA            | NA               | NA       |
| Lower Explosivity Level (LEL; unitless)                  | NA             | NA            | NA               | NA       |
| Critical Temperature (K)                                 |                | NR            | NA               | NA       |
| Enthalpy of Vaporization (cal/mol)                       |                | NR            | NA               | NA       |
| Density (g/mL, g/cm <sup>3</sup> )                       |                | NR            | NA               | NA       |
| EMSOFT Flux Residential 2 m (mg/day/cm <sup>2</sup> )    | NA             | NR            | EMSOFT           | NA       |
| EMSOFT Flux Residential 5 m (mg/day/cm <sup>2</sup> )    | NA             | NR            | EMSOFT           | NA       |
| EMSOFT Flux Nonresidential 2 m (mg/day/cm <sup>2</sup> ) | NA             | NR            | EMSOFT           | NA       |
| EMSOFT Flux Nonresidential 5 m (mg/day/cm <sup>2</sup> ) | NA             | NR            | EMSOFT           | NA       |

**(B) Toxicity Values/Benchmarks**

|   | Part 201 Value   | Updated Value   | Source/Reference/Date | Comments/Notes/Issues |
|---|--|---|-----------------------|-----------------------|
| <b>Reference Dose (RfD) (mg/kg/day)</b> | 1.6E+0   | 1.6E+0  | IRIS, 1991            |                       |
| <b>RfD details</b>                      | <p>NOAEL = 10 mg nitrate-nitrogen/l; LOAEL = 1.8 - 3.2 mg/kg/d; Critical effects = early signs of methemoglobine mia in excess of 10%; Human epidemiological study (Bosch et al., 1950; Walton, 1951). Babies 3-10 months old, formula administered; UF = 1. RfD not used for DCC because it is inappropriate (unlikely that 3-10 month baby would be outside playing in dirt). 8/22/1990 IRIS</p> | <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></p> <ol style="list-style-type: none"> <li>1. Bosch, H.M., A.B. Rosefield, R. Huston, H.R. Shipman and F.L. Woodward. 1950. Methemoglobinemia and Minnesota well supplies. J. Am. Water Works Assoc. 42: 161-170.</li> <li>2. Walton, G. 1951. Survey of literature relating to infant methemoglobinemia due to nitrate-contaminated water. Am. J. Public Health. 41: 986-996.</li> </ol> <p><b>Methods:</b> Bosch et al. (1950) evaluated 139 cases of cyanosis due to methemoglobinemia reported by physicians in Minnesota. All of the cases were in young children (ages 8 days to 5 months), with 90% occurring in infants &lt;2 months of age. A study of the nitrate concentration of the wells (a total of 129) used to supply water to the children with methemoglobinemia was performed. None of the wells contained &lt;10 mg/L nitrate-nitrogen. Two wells (1.5%) contained 10- 20 mg/L, although the diagnosis of methemoglobinemia was considered questionable in both these cases. There were 25 wells (19%) that contained 21-50 mg/L, 53 (41%) that contained 51-100 mg/L, and 49 (38%) that contained &gt;100 mg/L nitrate-nitrogen. Walton (1951) described a survey performed by the American Public Health Association to identify clinical cases of infantile methemoglobinemia that were associated with ingestion of nitrate-contaminated water. A total of 278 cases of methemoglobinemia were reported. Of 214 cases for which data were available on nitrate levels in water, none occurred in infants consuming water containing &lt;10 mg nitrate-nitrogen/L (1.6 mg nitrate-nitrogen/kg/day). There were 5 cases (2%) in infants exposed to 11-20 mg nitrate-nitrogen/L (1.8-3.2 mg/kg/day), 36 cases (17%) in infants exposed to 21-50 mg/L (3.4-8.0 mg/kg/day), and 173 (81%) in infants exposed to &gt;50 mg/L (&gt;8 mg/kg/day). Data on the ages of the infants</p> |                       | Complete              |



|  | Part 201 Value | Updated Value   | Source/Reference/Date | Comments/Notes/Issues |
|--|----------------|---|-----------------------|-----------------------|
|  |                | <p>were not provided.<br/> <b>Critical effect:</b> Methemoglobinemia.<br/> <b>End point or Point of Departure (POD):</b> NOAEL = 10 mg nitrate-nitrogen/L (1.6 mg/kg/day)<br/>                     Note: The studies of Bosch et al. (1950) and Walton (1951) provide convincing evidence that infantile methemoglobinemia does not occur at drinking water levels of 10 mg nitrate-nitrogen/L or less. This is supported by a large number of additional epidemiological and case studies in humans (e.g., Cornblath and Hartmann, 1948; Simon et al., 1964; Toussaint and Selenka, 1970; Craun et al., 1981; see U.S. EPA, 1990 for descriptions of additional studies).<br/> <b>Uncertainty Factors:</b> UF = 1 because available data define the NOAEL for the critical toxic effect in the most sensitive human subpopulation.<br/> <b>Source and date:</b> IRIS, 10/1/1991.</p> <p><b>EPA-OPP (1991):</b> Includes sodium nitrate (7631-99-4) and Potassium Nitrate (7757-79-1). No RfD or cPAD values listed. Data more recent or relevant than the information in IRIS is not presented in this document.</p> <p><b>Tier 2 Sources:</b><br/> <b>PPRTV:</b> No PPRTV record available at this time.<br/> <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b><br/> <b>MDEQ:</b> DEQ-CCD/-WRD, 9/30/2003. The drinking water HNV was based on a NOAEL of 10 mg nitrate-nitrogen (1.6 mg/kg/d) in 0-3 month old infants exposed to nitrates in water used to prepare formula (Bosch et al., 1950; Walton, 1951). An uncertainty factor of 1 was used since the key study was in a sensitive age group of humans.</p> |                       |                       |
| Oral Cancer Slope Factor (CSF) (mg/kg-day) <sup>-1</sup> | NA             | NA  | MDEQ, 2015            |                       |
| CSF details  | --             | <p><b>Tier 1 and Sources:</b><br/> <b>IRIS:</b> Per IRIS 10/1/1991, no value available.</p>   |                       | Complete              |



|  | Part 201 Value | Updated Value   | Source/Reference/Date | Comments/Notes/Issues |
|--|----------------|---|-----------------------|-----------------------|
|  |                | <p><b>PPRTV:</b> No PPRTV record available at this time.<br/> <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 values Source:</b><br/> <b>MDEQ:</b> Per DEQ-CCD, no value available.</p>  |                       |                       |
| Reference Concentration (RfC) or Initial Threshold Screening Level (ITSL) ( $\mu\text{g}/\text{m}^3$ ) | NA             | NA  | MDEQ, 2015            |                       |
| RfC/ITSL details   | --             | <p><b>Tier 1 and 2 Sources:</b><br/>                     Per IRIS 10/1/1991, no value available.<br/> <b>PPRTV:</b> No PPRTV record available at this time.<br/> <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b><br/> <b>MDEQ:</b> Per DEQ-CCD, record available at this time.</p>     |                       | Complete              |
| Inhalation Unit Risk Factor (IURF) ( $(\mu\text{g}/\text{m}^3)^{-1}$ )                                 | NA             | NA  | MDEQ, 2015            |                       |
| IURF details   | --             | <p><b>Tier 1 and 2 Sources:</b><br/> <b>IRIS:</b> Per IRIS 10/1/1991, record available at this time.<br/> <b>PPRTV:</b> No PPRTV record available at this time.<br/> <b>MRL:</b> No MRL record available at this time.</p> <p><b>Tier 3 Source:</b><br/> <b>MDEQ:</b> Per DEQ-CCD, record available at this time.</p> |                       | Complete              |
| 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. Per EPA-OPP (1991); Both sodium nitrate and potassium nitrate are reported to cause mutagenic affects in various genetic toxicity tests (Sax, N. I., and Lewis, R.   |                       |                       |



|  | Part 201 Value | Updated Value  | Source/Reference/<br>Date      | Comments/Notes<br>/Issues |
|--|----------------|--|--------------------------------|---------------------------|
|  |                | J. SR (1989) Dangerous Properties of Industrial Materials, 7th Edition. Van Nostrand Reinhold, New York and Ishidate, M. Jr., and Odashima, S. (1977) Mutation Research 48:337-354 |                                |                           |
| <b>Developmental or Reproductive Effector? (Y/N)</b>     | No             | Yes-oral. The RfD is based on a reproductive-developmental effect.<br>Oral Exposure Pathways-Full Term Exposure  | MDEQ, 2015                     |                           |
| <b>Developmental or Reproductive Toxicity Details</b>    | NA             | See IRIS file and info for the RfD above.  |                                |                           |
| <b>State Drinking Water Standard (SDWS) (µg/L)</b>       | --             | 1.0E+4   | 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   | 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  |                                |                           |
| <b>Is there an Aesthetic Value? (Y/N)</b>                | NO             | Not evaluated.   | NA                             |                           |
| <b>Aesthetic value details</b>                           | NA             | NA   |                                |                           |
| <b>Is there a Phytotoxicity Value? (Y/N)</b>             | NO             | Not evaluated.   | NA                             |                           |
| <b>Phytotoxicity details</b>                             | NA             | NA   |                                |                           |
| <b>Others:</b>   |                |  |                                |                           |

**(C) Chemical-specific Absorption 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, 2004 |                           |
| ABS <sub>gi</sub> details   |                | RAGS E (USEPA, 2004) Default Value |                               |                           |
| Skin absorption efficiency value (AE <sub>d</sub> )               | ---            | 0.01                               | MDEQ, 2015                    |                           |
| AE <sub>d</sub> details   |                |                                    |                               |                           |
| Ingestion Absorption Efficiency (AE <sub>i</sub> )                |                | 0.5                                | MDEQ, 2015                    |                           |
| AE <sub>i</sub> Details   |                |                                    |                               |                           |
| Relative Source Contribution for Water (RSC <sub>w</sub> )        |                | 1.0                                | 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> | 10,000 |

|  | <b>Rule 57 Value (µg/L)</b> | <b>Verification Date</b> |
|--|-----------------------------|--------------------------|
| <b>Human Non-cancer Values- Drinking water source (HNV-drink)</b>          | 10,000                      | 9/2003                   |
| <b>Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink)</b> | NLS                         | NA                       |
| <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>   | NLS                         | NA                       |
| <b>Aquatic maximum value (AMV)</b>   | NLS                         | NA                       |
| <b>Final Acute Value (FAV)</b>   | NLS                         | NA                       |

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> | 100          | 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     |