



CHEMICAL UPDATE WORKSHEET

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|-----------------------|--------------------------------------|
| Chemical Name: | p-Chlorobenzene sulfonic acid |
| CAS #: | 98-66-8 |
| 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) | 192.62 | 192.62 | EPI | EXP |
| Physical State at ambient temp | Solid | Solid | MDEQ | |
| Melting Point (°C) | 76 | 67.00 | EPI | EXP |
| Boiling Point (°C) | 300 | NA | NA | |
| Solubility (ug/L) | NA | 3.06300E+08 | PP | EST |
| Vapor Pressure (mmHg at 25°C) | NA | 4.28E-06 | PP | EST |
| HLC (atm-m ³ /mol at 25°C) | NA | 1.86E-09 | PP | EST |
| Log Kow (log P; octanol-water) | -0.52 | -0.52 | PP | EST |
| Koc (organic carbon; L/Kg) | 4.64E-1 | 16.06 | EPI | EST |
| Ionizing Koc (L/kg) | | NR | NA | NA |
| Diffusivity in Air (Di; cm ² /s) | NA | 5.70E-02 | W9 | EST |
| Diffusivity in Water (Dw; cm ² /s) | NA | 6.6561E-06 | W9 | EST |
| Soil Water Partition Coefficient (Kd; inorganics) | NR | NR | NA | NA |

| | Part 201 Value | Updated Value | Reference Source | Comments |
|----------------------------------------------------------|----------------|---------------|------------------|----------|
| Flash Point (°C) | 226 F | NA | NA | NA |
| Lower Explosivity Level (LEL; unitless) | NA | NA | NA | NA |
| Critical Temperature (K) | | NA | NA | NA |
| Enthalpy of Vaporization (cal/mol) | | NA | NA | NA |
| Density (g/mL, g/cm ³) | | NA | NA | NA |
| EMSOFT Flux Residential 2 m (mg/day/cm ²) | NA | 7.80E-07 | EMSOFT | EST |
| EMSOFT Flux Residential 5 m (mg/day/cm ²) | NA | 7.80E-07 | EMSOFT | EST |
| EMSOFT Flux Nonresidential 2 m (mg/day/cm ²) | NA | 9.59E-07 | EMSOFT | EST |
| EMSOFT Flux Nonresidential 5 m (mg/day/cm ²) | NA | 9.59E-07 | 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+0 | 8.0E-1 | CALEPA, 2015/MDEQ, 2015 | |
| RfD details | Administered to male and female rodents by oral gavage for 28 days. 10 male and 10 female rats per group. Dose groups: 0, 10, 50, 500, 1,000 and 2,000 mg/kg of p-CBSA. Study conducted under EPA contract by American Biogenecis Corp. NOAEL for females = 2,000 mg/kg. Two high-dose males had slightly lower body weights and exhibited salivation, gasping and irregular breathing. The NOAEL for males equal to or greater than 1,000 mg/kg. UF | <p>Tier 3 Source: CALEPA: Basis: CAL OEHHA derived a RfD of 0.266 mg/kg-day based on the same key study used by MDEQ but used a BMDL of 797 mg/kg-day of in place of NOAEL and a higher UF of 3,000. MDEQ adopted the BMDL value and applied a UF of 1,000 to derive a RfD of 8.0E-1 mg/kg-day. See details below.</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (7/07/2009), no value at this time. PPRTV identified only one toxicity study: Kryatov, I.A. 1970. Hygienic evaluation of sodium p-chlorobenzene sulfonate and chloral as water pollutant. Hyg. Sanit. 35:333–338. (English translation from Gig. Sanit.). This subchronic study administered 0, 0.1, 1.0, or 10 mg/kg-day of p-chlorobenzene sulfonic acid orally to rabbits for 7 months. Per PPRTV, Kryatov (1970) did not present enough details pertaining to methods and results to allow for the derivation of a provisional toxicity value and no other studies regarding oral exposure of animals to p-chlorobenzene sulfonic acid are available. MRL: No MRL record available at this time.</p> <p>Tier 3 Sources: MDEQ: DEQ/RRD (2005) RfD = 1.0E+0 mg/kg-day: Critical Study (ies): American Biogenics Corporation. 1985. Final Report for American Biogenics Corporation Study 410-2298. Twenty-eight Day Oral (gavage) Toxicity Study in Albino Rats using A-100. Study conducted under EPA contract.(unpublished) Method(s): rats (10/sex/dose group) were exposed to 0, 10, 50, 500, 1,000 and 2,000 mg/kg p-CBSA oral gavage for 28 days. Critical effect: lower body weights, salivation, gasping and irregular breathing.</p> | | Complete |



| | Part 201 Value | Updated Value | Source/Reference/Date | Comments/Notes/Issues |
|--|------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|-----------------------|
| | <p>= 1,000 [10 (intraspecies) X 10 (interspecies) X 10 (subchronic to chronic). RfD = 1.0 mg/kg-day. CCD/RRD date: 11/15/2005.</p> | <p>End point or Point of Departure (POD): NOAEL = 1,000 mg/kg-day Uncertainty Factors: UF = 1,000 (10 each for intraspecies variability, interspecies extrapolation and use of a subchronic study.) Source and date: DEQ/RRD, 11/15/2005.</p> <p>California DTSC/OEHHA (CALEPA): RfD= 0.266 (mg/kg/day). OEHHA used the Benchmark Dose (BMD) software to estimate the point of departure (POD) as BMD modeling provides a more quantitative approach to deriving a POD versus the traditional NOAEL approach. <u>Derivation process:</u> Key Study: American Biogenics Corporation (1985). Twenty-eight day oral (gavage) toxicity study in albino rats using A-100 (4-Chlorobenzenesulfonic acid). Decatur, IL. Methods: male and female Sprague-Dawley rats (10/sex/dose group) were dosed by gavage at 0, 10, 50, 500, 1000, or 2000 mg/kg-day for 31 or 32 days. This study is also referred to as the 28-day rat toxicity study to retain consistency with previous documents that cite this study for determining reference levels (DTSC, 1997; MDEQ, 2006). POD: BMDL1SD = 797 mg/kg-day Chronic UF: for chronic exposure – 3,000 (10 for interspecies extrapolation, 30 for intraspecies variability, and 10 for sub chronic to chronic exposure). Chronic ADD: 0.266 mg/kg-day Note: OEHHA derived an acute ADD of 0.797 mg/kg-day based on the same BMDL value and a UF of 1,000 (10 for interspecies extrapolation, 30 for intraspecies variability, and 10 for sub chronic to chronic exposure). Source: OEHHA. Public Health Protective Concentration. para-Chlorobenzene Sulfonic Acid in Drinking Water, 2/2015</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 Massachusetts, Minnesota, New Jersey, New York and Texas, WHO (IARC), WHO (IPCS/INCHEM), Canada, The Netherlands (RIVM), ECHA (REACH) and OECD HPV.</p> | | |



| | Part 201 Value | Updated Value | Source/Reference/Date | Comments/Notes/Issues |
|------------------------------------------------------------------------------------------------|----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|-----------------------|
| Oral Cancer Slope Factor (CSF) (mg/kg-day ⁻¹) | -- | NA | MDEQ, 2015 | |
| CSF details | NA | <p>Carcinogen Weight-of-Evidence (WOE) Class: "Inadequate Information to Assess the Carcinogenic Potential"</p> <p>IRIS WOE Basis: Studies evaluating the carcinogenic potential of oral or inhalation exposure to p-CBSA in humans or animals were not identified in the available literature.</p> <p>Source and Date: PPRTV, 7/07/2009</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (7/07/2009), no value 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/m ³) | -- | NA | MDEQ, 2015 | |
| RfC/ITSL details | NA | <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (7/07/2009), no value at this time. MRL: No MRL record available at this time.</p> <p>Tier 3 Source: MDEQ: Per DEQ-CCD, no value at this time.</p> | | Complete |
| Inhalation Unit Risk Factor (IURF) ((µg/m ³) ⁻¹) | -- | NA | MDEQ, 2015 | |



| | Part 201 Value | Updated Value | Source/Reference/Date | Comments/Notes/Issues |
|---------------------------------------------------|----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------|-----------------------|
| IURF details | NA | <p>Carcinogen Weight-of-Evidence (WOE) Class: "Inadequate Information to Assess the Carcinogenic Potential"</p> <p>IRIS WOE Basis: Studies evaluating the carcinogenic potential of oral or inhalation exposure to p-CBSA in humans or animals were not identified in the available literature.</p> <p>Source and Date: PPRTV, 7/07/2009</p> <p>Tier 1 and 2 Sources: IRIS: No IRIS file available at this time. PPRTV: Per PPRTV (7/07/2009), no value 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 |
| Mutagenic Mode of Action (MMOA)? (Y/N) | -- | NO | USEPA, 2014 | |
| MMOA Details | -- | NA Not listed as a carcinogen with mutagenic MOA in the USEPA OSWER List. | | |
| Developmental or Reproductive Effector? (Y/N) | No | No, the RfD is not based on a reproductive-developmental effect. | MDEQ, 2014 | |
| 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 | |



| | Part 201 Value | Updated Value | Source/Reference/ Date | Comments/Notes /Issues |
|--------------------------------------------------------------|----------------|-------------------------------------------------------------------------|---------------------------|---------------------------|
| SMCL details | NA | MI Safe Drinking Water Act (SDWA) 1976 PA 399 and USEPA SMCL List, 2015 | | |
| Is there an aesthetic value for drinking water? (Y/N) | NO | Not evaluated. | NA | |
| Aesthetic value (ug/L) | NO | 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 (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) | ID |
| Updated GSI value (µg/L) | ID |
| Rule 57 Drinking Water Value (µg/L) | 28,000 |

| | Rule 57 Value (µg/L) | Verification Date |
|----------------------------------------------------------------------------|-----------------------------|--------------------------|
| Human Non-cancer Values- Drinking water source (HNV-drink) | 28,000 | 8/2009 |
| Human Non-Cancer Values- Non-drinking water sources (HNV-Non-drink) | 2,200,000 | 8/2009 |
| 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) | ID | 8/2009 |
| Aquatic maximum value (AMV) | ID | 8/2009 |
| Final Acute Value (FAV) | ID | 8/2009 |

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 ($\mu\text{g}/\text{kg}$) | 200 | MDEQ, 2015 |
| Target Detection Limit – Water ($\mu\text{g}/\text{L}$) | 10 | MDEQ, 2015 |
| Target Detection Limit – Air (ppbv) | NA | MDEQ, 2015 |
| Target Detection Limit – Soil Gas (ppbv) | 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 |

