

Rule 57 Aquatic Values Data Sheet

8/25/2010

Chemical or product name: 4-Chlorophenol

Manufacturer (WTAs): -----

C.A.S #: 106-48-9

Developed by: Christopher Hull FAV*: 530 ug/l

Approved by: D. Bush AMV*: 270 ug/l

Approval date: 10/4/2010 FCV*: 30 ug/l

CAS: 12/17/09; AQUIRE: 12/14/09; QSAR: 6/22/09 Acute CF: ----

Clearinghouse search date: -----

(Tier: II)

(Tier: II)

(Tier: II)

Chronic CF: ----

ACUTE DATA

| Species | Endpoint (EC or LC50) | Duration (hours) | Test Type (FT,M, etc.) | Hardness mg/L | Test Chemical | LC50/EC50 ug/L | SMAV ug/L | GMAV ug/L | Rank | Reference |
|--------------------------------|--------------------------|---------------------|---------------------------|------------------|------------------|--------------------|--------------|--------------|------|-----------|
| Water Flea | LC50 | 48 | S,U | 173 | ----- | 4,100 ¹ | 4,252 | 4,252 | 1 | 1 |
| (<i>Daphnia magna</i>) | LC50 | 48 | S,U | 150 | ----- | 4,410 ¹ | | | | 2 |
| Fathead Minnow | EC50 | 96 | FT,M | 44.8 | ----- | 5,710 | 5,710 | 5,710 | 2 | 3 |
| (<i>Pimephales promelas</i>) | LC50 | 96 | FT,M | 45 | ----- | 6,110 ² | | | | 3 |
| Pink Hydra | LC50 | 96 | S,M | ----- | ----- | 32,000 | 32,000 | 37,947 | 3 | 4 |
| (<i>Hydra vulgaris</i>) | | | | | | | | | | |
| Green Hydra | LC50 | 96 | S,M | ----- | ----- | 45,000 | 45,000 | | | 4 |
| (<i>H. viridissima</i>) | | | | | | | | | | |

CHRONIC DATA

| Species | Test type (ELS, etc.) | Duration (days) | Study Conditions (FT,M etc.) | Hardness mg/L | Test Chemical | MATC ug/L | SMCV ug/L | GMCV ug/L | Rank | Reference |
|---------|--------------------------|--------------------|------------------------------------|------------------|------------------|--------------|--------------|--------------|------|-----------|
|---------|--------------------------|--------------------|------------------------------------|------------------|------------------|--------------|--------------|--------------|------|-----------|

- NO SUITABLE DATA WERE FOUND.

*Value rounded to 2 significant figures.

¹ Lyman et al. (1982; p. 15-15) would conclude that a chemical with these properties will volatilize at significant rates in open water (QSAR, 6/22/10). Therefore, data from tests with measured concentrations should be preferred.

² This value was not used to calculate the SMAV, because an EC50 value from the same test is preferred and available.

| Min. Data Req. met | Acute Factor |
|-----------------------|-----------------|
| 2 | 13 |
| 3 | 8 |
| 4 | 7 |
| 5 | 6.1 |
| 6 | 5.2 |
| 7 | 4.3 |

RULE 57 AQUATIC VALUES WORK SHEET-ACUTE

Chemical Name: 4-Chlorophenol

CAS #: 106-48-9

Developed by: Christopher Hull

Date: 8/25/10

AQUATIC MAXIMUM VALUE CALCULATIONS

A. Minimum 8-species requirement for Tier I is **not** met (Tier II): Yes.

1. Minimum requirements met = 3 (iii, iv, vii).

2. Minimum requirements missing for Tier I = 5 (i, ii, v, vi, viii).

3. Acute Factor = 8.

4. Toxicity is **not** dependent upon a water quality characteristic: Yes.

a. FAV calculation: Tier II FAV = Lowest GMAV / Acute Factor = $4,252 \text{ ug/l} / 8 = \underline{531.5 \text{ ug/l}}$.

5. Toxicity is dependent upon a water quality characteristic: No.

a. Slope = _____ (Table _____).

b. FAV equation: Tier II FAV = _____ = _____ = _____.

6. Go to C.

B. Minimum 8-species requirement is met (Tier I): No.

1. Toxicity is **not** dependent upon a water quality characteristic: _____.

a. Tier I FAV calculation: _____ (_____).

2. Toxicity is dependent upon a water quality characteristic: _____.

a. Slope = _____ (Table _____).

b. Ranked genus mean acute intercepts: Table _____.

c. Final acute intercept = _____ (_____).

ln of final acute intercept = _____.

d. FAV equation: Tier I FAV = _____ = _____ = _____.

C. Aquatic Maximum Value (AMV) calculation: Tier II AMV = $\text{Tier II FAV} / 2 = 531.5 \text{ ug/l} / 2 = \underline{265.75 \text{ ug/l}}$.

RULE 57 AQUATIC VALUES WORK SHEET-CHRONIC

Chemical Name: 4-Chlorophenol

CAS #: 106-48-9

Developed by: Christopher Hull

Date: 8/25/10

FINAL CHRONIC VALUE CALCULATIONS

A. Minimum 8-species requirement for GMCV-based Tier I is not met: Yes.

1. Minimum requirements met = 0.
2. Minimum requirements missing = 8.

B. Minimum 8-species requirement for GMCV-based Tier I is met: No.

1. Toxicity is **not** dependent upon a water quality characteristic: _____.
 - a. Tier I FCV = _____ (Fig. _____).
2. Toxicity is dependent upon a water quality characteristic: _____.
 - a. Slope = _____ (Table _____).
 - b. Ranked Genus Mean Chronic Intercepts: Table _____.
 - c. Final Chronic Intercept = _____ (Fig. _____).
 - d. ln of Final Chronic Intercept = _____.
 - e. FCV equation = Tier I FCV = _____ = _____ = _____.

C. Acute-to-Chronic-Ratio method: Yes.

1. Acute-to-Chronic Ratio:
 - a. Number of ACRs meeting minimum data requirements = 0 (Table-----).
 - b. Tier II Acute-to-Chronic Ratio = Default Value = $Xg(18, 18, 18) = 18$.

2. Toxicity is **not** dependent upon a water quality characteristic: Yes.

$$\text{Tier II FCV} = \text{Tier II FAV} / \text{Tier II ACR} = 531.5 \text{ ug/l} / 18 = \underline{29.527778 \text{ ug/l}}$$

3. Toxicity is dependent upon a water quality characteristic: No.

- a. Slope = _____ (Table _____).
- b. Aquatic Chronic Intercept = _____ (Table _____).
- c. ln of Aquatic Chronic Intercept = _____.
- d. FCV equation = Tier _____ FCV = _____ = _____ = _____.

4-CHLOROPHENOL REFERENCES, 8/10

References Used:

1. #007906 : LeBlanc, G. A. 1980. Acute toxicity of Priority Pollutants to water flea (*Daphnia magna*). Bull. Environ. Contam. Toxicol. 24(5): 684-91 .
2. #019115: Kim, K. T., Lee, Y. G., and Kim, S. D. 2006. Combined toxicity of copper and phenol derivatives to *Daphnia magna*: effect of complexation reaction. Environ. Int 32(4): 487-492.
3. #QL 638 .C94 A27 v.5: Geiger, D. L., Brooke, L. T., and Call, D. J. 1990. Acute toxicities of organic chemicals to Fathead Minnows (*Pimephales promelas*), Volume 5. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI:332 .
4. #019180: Pollino, C. A. and Holdway, D. A. 1999. Potential of two *Hydra* species as standard toxicity test animals. Ecotoxicology and Environmental Safety 43(3): 309-316.

References Reviewed, but Not Used:

- #V1081: Abe, T., Saito, H., Nlikura, Y., Shigeoka, T., and Nakano, Y. 2000. Embryonic development assay with *Daphnia magna*: application to toxicity of chlorophenols. Water Sci. Technol. 42(7-8): 297-304.
-NUE; TDI.
- #SH 11 .A335 no.207: Applegate, V. C., Howell, J. H., Hall, A. E., and Smith, M. A., 1957. Toxicity of 4,346 chemicals to larval lampreys and fishes. Spec. Sci. Rep.-Fish. No. 207. Fish Wildl. Serv., U.S.D.I., Washington, D.C.:157 p.
-NUE.
- #V1090: Argese, E., Bettiol, C., Ghelli, A., Todeschini, R., and Miana, P. 1995. Submitochondrial particles as toxicity biosensors of chlorophenols. Environ. Toxicol. Chem. 14(3): 363-8.
-NUE.
- #V1012: Babich, H. and Borenfreund, E. 1987 . *In vitro* cytotoxicity of organic pollutants to Bluegill Sunfish (BF-2) cells. Environ. Res. 42(1): 229-37.
-NUE.
- #V1096: Bearden, A. P. and Schultz, T. W. 1998. Comparison of *Tetrahymena* and *Pimephales* toxicity based on mechanism of action. SAR QSAR Environ. Res. 9(3-4): 127-153.
-QSAR / SDO.
- #V1097: Bearden, A. P. and Schultz, T. W. 1997. Structure-activity relationships for *Pimephales* and *Tetrahymena*: a mechanism of action approach. Environ. Toxicol. Chem. 16(6): 1311-1317.
-QSAR / SDO.
- #Y2020: Beirat der Bundesraztekammer. 1989. Belastung der Bevlkerung durch Perchlorethylen. Deutsches Razteblatt 86, Heft 49: C2239-C2241.
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- #V1100: Benoit-Guyod, J. L., Andre, C., and Clavel, A. K. 1984. Chlorophenols: degradation and toxicity (Chlorophenols: Degradation et Toxicite). J Fr Hydrol 15(3): 249-266.
-NUE.
- #017541: Botsford, J. L. 2002. A comparison of ecotoxicological tests. Altern Lab Anim 30(5): 539-50.
-TONS; TMCU; or SDO.
- #V2039: Boyd, E. M., Killham, K., and Meharg, A. A. 2001. Toxicity of mono-, di- and tri-chlorophenols to lux marked terrestrial bacteria, *burkholderia* species Rasc c2 and *Pseudomonas fluorescens*. Chemosphere 43(2): 157-66.
-TONS.
- #007905: Buccafusco, R. J., Ells, S. J., and Leblanc, G. A. 1981. Acute toxicity of Priority Pollutants to bluegill (*Lepomis macrochirus*). Bull Environ Contam Toxicol 26(4): 446-452.
-TM/CU.
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- #V1119: Cash, G. G. and Clements, R. G. 1996. Comparison of structure-activity relationships derived from two methods for estimating octanol-water partition coefficients. SAR QSAR Environ. Res. 5(2): 113-124.
-QSAR / SDO.
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-SD; IITM/C.
- #V1149: Castano, A., Vega, M. M., and Tarazona, J. V. 1995. Acute toxicity of selected metals and phenols on RTG-2 and CHSE-214 fish cell lines. Bulletin of Environmental Contamination and Toxicology 55(2): 222-9.
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- #V3126: Chen, C. Y. and Lin, J. H. 2006. Toxicity of chlorophenols to *Pseudokirchneriella subcapitata* under air-tight test environment. Chemosphere 62(4): 503-9.
-PDO.
- #V1123: Chen, J., Feng, L., Zhao, Y., and Wang, L. 1996. Using theoretical solvatochromic parameters in prediction of acute toxicity of substituted aromatic compounds to aquatic organisms. Chin. Sci. Bull. 41(9): 740-743.
-QSAR / SDO.
- #V3094: Colombo, A., Benfenati, E., Karelson, M., and Maran, U. 2008. The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity. Chemosphere 72(5): 772-780.
-NUE; MOD/QSAR/SDO.
- #V3127: Costescu, A. and Diudea, M. 2006. QSTR study on Aquatic Toxicity against *Poecilia reticulata* and *Tetrahymena pyriformis* using Topological indices. Internet Electronic Journal of Molecular Design 5(2): 116-134.
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-QSAR / SDO; TDI.
- #016592: Devillers, J. and Chambon, P. 1986. Acute toxicity of chlorophenols to *Daphnia magna* and *Brachydanio rerio*. J. Fr. Hydrol. 17(2): 111-19.
-*D. magna*: TDI; TONNA, SD.
- #V1170: Devillers, J. and Chambon, P. 1988. A methodological framework for the early detection of drinking water pollutants. Chemosphere 17(9): 1647-54.
-NUE; TDI.
- #006950: Devillers, J., Chambon, P., Zakarya, D., Chastrette, M., and Chambon, R. 1987. A predictive structure-toxicity model with *Daphnia magna*. Chemosphere 16(6): 1149-63.
-QSAR/SDO.
- #V1180: Devillers, J., Meunier, T., and Chambon, P. 1985. Usefulness of the dosage-effect-time relation in ecotoxicology for determination of different chemical classes of toxicants. Tech. Sci. Munic 80(7-8): 329-334.
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-NUE; QSAR / SDO.
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- #V1236: Eldred, D. V., Weikel, C. L., Jurs, P. C., and Kaiser, K. L. E. 1999. Prediction of Fathead Minnow acute toxicity of organic compounds from molecular structure. Chem. Res. Toxicol. 12(7): 670-678.

-NUE; QSAR / SDO.

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-QSAR / SDO.

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-SD; NUE; PD.

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-MDO.

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-NUE.

#007904: Heitmuller, P. T., Hollister, T. A., and Parrish, P. R. 1981. Acute toxicity of 54 industrial chemicals to Sheepshead Minnows (*Cyprinodon variegatus*). Bull. Environ. Contam. Toxicol. 27(5): 596-604.

-SWDO; no chronic data with which to calculate ACR.

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-TM/CU; IITM/C these data are later reported in 012010 & 013981.

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-SED.

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- #V1418: Kaiser, K. L. E., Niculescu, S. P., and Schuurmann, G. 1997. Feed forward backpropagation neural networks and their use in predicting the acute toxicity of chemicals to the Fathead Minnow. Water Qual. Res. J. Can. 32(3): 637-657.
-NUE; SDO.
- #V1420: Kamlet, M. J., Doherty, R. M., Abraham, M. H., and Taft, R. W. 1988. Solubility properties in biological media. 12. Regarding the mechanism of nonspecific toxicity or narcosis by organic nonelectrolytes. Quant. Struct.-Act. Relat. 7(2): 71-8.
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- #V1421: Kanabur, V. V. and Sannadurgappa, D. 2001. Acute toxicity of phenol and cresol to a freshwater fish *Oreochromis mossambicus*. Environment and Ecology 19(4): 756-758.
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- #V3125: Kanabur, V. and Sangli, A. 1998. Acute toxicity of chlorophenol and cresol to a freshwater fish *Lepidocephalichthys guntea*. Environment and Ecology 16(2): 334-336.
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- #V1422: Karabunarliev, S., Mekenyan, O. G., Karcher, W., Russom, C. L., and Bradbury, S. P. 1996. Quantum-chemical descriptors for estimating the acute toxicity of substituted benzenes to the Guppy (*Poecilia reticulata*) and Fathead Minnow (*Pimephales promelas*). Quant. Struct.-Act. Relat. 15(4): 311-320.
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- #V1424: Kasokat, T., Nagel, R., and Ulrich, K. 1989. Metabolism of chlorobenzene and hexachlorobenzene by the Zebra Fish, *Brachydanio rerio*. Bull. Environ. Contam. Toxicol. 42(2): 254-61.
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-NUE.
- #V1477: Kobayashi, K., Oshima, Y., Hamada, S., and Taguchi, C. 1987. Studies on the induction of drug-metabolizing enzymes in fish and shellfish-II. Induction of phenol-sulfate conjugating activity by exposure to phenols and duration of its induced activity in Short-Necked Clam. Nippon Suisan Gakkaishi 53(11): 2073-6.
-NUE.
- #013449: Kopperman, H. L., Carlson, R. M., and Caple, R. 1974. Aqueous chlorination and ozonation studies. I. Structure-toxicity correlations of phenolic compounds to *Daphnia magna*. Chem.-Biol. Interact. 9(4): 245-51.
-TM/CU.
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- #V3132: Kramer, N. I., Hermens, J. L., and Schirmer, K. 2009. The influence of modes of action and physicochemical properties of chemicals on the correlation between in vitro and acute fish toxicity data. Toxicol In Vitro 23(7): 1372-9.
-QSAR / SDO.
- #V1432: Kuhn, R. 1988. Schadstoffwirkungen von Umweltchemikalien im Daphnien-Reproduktions-Test als Grundlage für die Bewertung der Umweltgefährlichkeit in Aquatischen Sys... Forschungsbericht .
-NUE.
- #010301: Kuhn, R. and Pattard, M. 1990. Results of the harmful effects of water pollutants to green algae (*Scenedesmus subspicatus*) in the Cell Multiplication Inhibition Test. Water Res. 24(1): 31-8.

-PDO.

#012430: Kuhn, R., Pattard, M., Pernak, K., and Winter, A. 1989. Results of the harmful effects of selected water pollutants (anilines, phenols, aliphatic compounds) to *Daphnia magna*. Water Res 23(4): 495-499.

-TM/CU.

#010310: Kuhn, R., Pattard, M., Pernak, K. D., and Winter, A. 1989. Results of the harmful effects of water pollutants to *Daphnia magna* in the 21 day reproduction test. Water Res. 23(4): 501-10.

-TM/CU.

#V2310: Kuiper, J. and Hanstveit, A. O. 1984. Fate and effects of 4-chlorophenol and 2,4-dichlorophenol in marine plankton communities in experimental enclosures. Ecotoxicol. Environ. Saf. 8(1): 15-33.

-SW; PDO.

#019189: Lammer, E., Carr, G. J., Wendler, K., Rawlings, J. M., Belanger, S. E., and Braunbeck, T. 2009. Is the fish embryo toxicity test (FET) with the Zebrafish (*Danio rerio*) a potential alternative for the fish acute toxicity test? Comp Biochem Physiol C Toxicol Pharmacol 149(2): 196-209.

-Acute: SD, NA; Chronic: no test methods available, TDI for ELS tests.

#009664: LeBlanc, G. A. 1984. Interspecies relationships in acute toxicity of chemicals to aquatic organisms.

Environ. Toxicol. Chem. 3(1): 47-60.

-REJECT (SW; IITM/C). Possibly the same tests described in #OTS0517186.

#013412: LeBlanc, G. A., Hilgenberg, B., and Cochrane, B. J. 1988. Relationships between the structures of chlorinated phenols, their toxicity, and their ability to induce glutathione S-transferase activity in *Daphnia magna*.

Aquat. Toxicol. 12(2): 147-55.

-REJECT (TDI; ND for phenol; SDO).

#018359, #V2859: Lee, Y. G., Hwang, S. H., and Kim, S. D. 2006. Predicting the toxicity of substituted phenols to aquatic species and its changes in the stream and effluent waters. Archives of environmental contamination and toxicology 50(2): 213-9.

-IITM/C; TONNA; PD.

#V2809: Lipnick, Robert L., Bickings, Charlene K., Johnson, David E., and Eastmond, David A., 1985.

Comparison of QSAR predictions with fish toxicity screening data for 110 phenols ASTM Spec. Tech. Publ.

- QSAR / SDO.

#SH 157.7 .M241: MacPhee, C. and Ruelle, R. 1969. Lethal effects of 1888 chemicals upon four species of fish from Western North America : 112p.

-TDI.

#V1535: Martin, T. M. and Young, D. M. 2001 . Prediction of the acute toxicity (96-h LC50) of organic compounds to the Fathead Minnow (*Pimephales promelas*) using a Group Contribution method. Chem Res Toxicol 14(10): 1378-85.

-NUE; QSAR / SDO.

#007917: Mayes, M. A. , Alexander, H. C., and Dill, D. C. 1983. A study to assess the influence of age on the response of Fathead Minnows in static acute toxicity tests. Bull. Environ. Contam. Toxicol. 31(2): 139-147.

-TM/CU (low D.O.); IITM/C.

#V1542: McCarty, L. S., Hodson, P. V., Craig, G. R., and Kaiser, K. L. E. 1985. The use of Quantitative Structure-Activity Relationships to predict the acute and chronic toxicities of organic chemicals to fish. Environ. Toxicol.

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-QSAR / SDO.

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*For abbreviations used, see appendix; attached.

APPENDIX: REFERENCE ABBREVIATIONS USED, 8/10

AMD = ambient monitoring data.
BCF = bioconcentration factor.
D = data (as a suffix to other abbreviations listed here).
DEP = depuration data.
DO = data only (as a suffix to other abbreviations listed here).
EF = environmental fate.
FLO = foreign language, only.
GWD = groundwater data.
IITM/C = insufficient information on test methods / conditions.
ISD = *in situ* data.
LD = leachate data.
LSER = Linear Solvation Energy Relationship.
MCD = microcosm data.
MIX = mixture (not chemical-specific) test data.
MED = model ecosystem data.
MET = metabolism
MOD = model (theoretical) data / analysis.
NA = not available at this time.
ND = no data (on this chemical).
NIL = not in (MDEQ) Library.
NR = not reviewed.
NUE = no useable endpoint.
O = only (as a suffix to other abbreviations listed here).
PD = phytotoxicity data.
PHYS = physiological data.
QSAR = Quantitative Structure-Activity Relationship.
RWD = receiving water data.
SD = secondary data.
SED = sediment data or testing.
SW = saltwater.
TATO = test animals too old.
TDI = test duration inappropriate.
TM/CU = test methods / conditions unacceptable.
TONNA = test organisms not North American.
TONS = test organisms not suitable.
TTD = time-toxicity data.
UD or UP = uptake data.
WET = whole-effluent testing.