

Rule 57 Aquatic Values Data Sheet

6/5/2006

Chemical or product name: 2-Chlorophenol

Manufacturer (WTAs): -----

C.A.S #: 95-57-8

Developed by: Christopher Hull FAV*: 320 ug/l

Approved by: D. Bush

Approval date: 6/30/08

CAS, AQUIRE: 2/14/06

Clearinghouse search date: 6/20/96

AMV*: 160 ug/l

FCV*: 18 ug/l

Acute CF: ----

Chronic CF: ----

(Tier: II)

(Tier: II)

(Tier: II)

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 (<i>Daphnia magna</i>)	LC50	48	S,U	173	-----	2,600	2,600	2,600	1	1
Bluegill Sunfish (<i>Lepomis macrochirus</i>)	LC50	96	S,U	20	-----	10,000	9,165	9,165	2	2
	LC50	96	S,U	20	-----	8,400				3
Fathead Minnow (<i>Pimephales promelas</i>)	LC50	96	FT,M	45.9	-----	11,000	11,614	11,614	3	4
	LC50	96	FT,M	45.9	-----	13,000				4
	LC50	96	FT,M	44.9	-----	13,800				5
	EC50	96	FT,M	42.6	-----	9,220				6
	LC50	96	FT,M	42.6	-----	9,410 ¹				6,7 ²
	LC50	96	S,U	20	-----	11,630 ³				2
	LC50	96	S,U	360	-----	14,480 ³				2
Goldfish (<i>Carassius auratus</i>)	LC50	96	S,U	20	-----	12,370	12,370	12,370	4	2
Guppy (<i>Poecilia reticulata</i>)	LC50	96	S,U	20	-----	20,170	20,170	20,170	5	2

(cont'd.)

9/21/04

CHRONIC DATA

Page 2

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

NO SUITABLE DATA WERE FOUND.

*Value rounded to 2 significant figures.

¹ Value not used for calculation of SMAV because EC50 preferred over LC50 from the same test.

² This reference reports a slightly different hardness for this test, due to differences in calculation.

³ Value not used for calculation of SMAV because FT,M data preferred over data from other test types.

9/21/04

CHRIS FALL

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

Chemical Name: 2-Chlorophenol
 C.A.S. #: 95-57-8

AQUATIC MAXIMUM VALUE CALCULATIONS, 6/06

- A. Minimum 8 species requirement is **not** met (Tier II). Minimum requirements met = 3
 Minimum requirements missing for Tier I = 5 (i, v, vi, vii, viii) -
 Acute factor = 8 -

1. Toxicity is **not** dependent on a water characteristic

a. FAV calculation $FAV = \frac{\text{lowest } \Sigma MAU}{\text{Acute Factor}} = \frac{2,600 \mu g/l}{8} = \boxed{325 \mu g/l}$

2. Toxicity is dependent on a water characteristic

a. Slope = (Table)

b. FAV equation:

3. Go to C.

- B. Minimum 8 species requirement **is** met (Tier I)

1. Toxicity is **not** dependent on a water characteristic

a. FAV calculation: Att.

2. Toxicity is dependent on a water characteristic

a. Slope = (Table)

b. Ranked genus mean acute intercepts: Table

c. Final acute intercept = (Att.)

ln of final acute intercept =

d. FAV equation =

C. Aquatic Maximum Value (AMV) calculation: $AMV = \frac{FAV}{2} = \frac{325 \mu g/l}{2} = \boxed{162.5 \mu g/l}$

2-CHLOROPHENOL:

Chris Hall

FINAL CHRONIC VALUE CALCULATIONS, 6/06

A. Minimum 8 species requirement is not met (Tier II). Minimum requirements met = 0
Minimum requirements missing for Tier I = 8

1. Acute to chronic ratio

a. Number ACRs meeting minimum data requirements = 0 (Table —)

b. Acute to chronic ratio = 18

2. Toxicity is **not** dependent on a water characteristic

$$FCV = \frac{FAU}{ACR} = \frac{325 \text{ } \mu\text{g/L}}{18} = \boxed{18.055556 \text{ } \mu\text{g/L}}$$

3. Toxicity is dependent on a water characteristic

a. Slope = (Table —)

b. Aquatic chronic intercept = (Table —)

ln of aquatic chronic intercept =

c. FCV equation =

B. Minimum 8 species requirement is met (Tier I)

1. Toxicity is **not** dependent on a water characteristic

a. FCV = — (Att. —)

2. Toxicity is dependent on a water characteristic

a. Slope = (Table —)

b. Ranked genus mean chronic intercepts: Table —

c. Final chronic intercept = — (Att. —); ln of final chronic intercept =

d. FCV equation =

2-CHLOROPHENOL REFERENCES, 5/06

References Used:

1. #007906: LeBlanc, Gerald A. 1980. Acute toxicity of Priority Pollutants to water flea (*Daphnia magna*). Bull. Environ. Contam. Toxicol. 24(5): 684-91.
2. #004630: Pickering, Q. H. and Henderson, C. 1966. Acute toxicity of some important petrochemicals to fish. J. Water Pollut. Control Fed. 38(9): 1419-1429.
3. #004613: Henderson, C.; Q.H. Pickering; and A.E. Lemke. 1961. The effect of some organic cyanides (nitriles) on fish. Proc. 15th Ind. Waste Conf., Eng. Bull. Purdue Univ., Ser. No. 106, 65(2): 120-130.
4. #009059: Phipps, Gary L., Holcombe, Gary W., and Fiandt, James T. 1981. Acute toxicity of phenol and substituted phenols to the Fathead Minnow. Bull. Environ. Contam. Toxicol. 26(5): 585-93.
5. #QL 638 .C94 A27 v.2: Geiger, D. L., Northcott, C. E., Call, D. J., and Brooke, L. T. 1985. Acute toxicities of organic chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 2. Center for Lake Superior Environmental Stud., Univ. of Wisconsin-Superior, Superior, WI 1:326.
6. #QL 638 .C94 A27 v.4: Geiger, D. L., Call, D. J., and Brooke, L. T. 1988. Acute toxicities of organic chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 4. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI:355.
7. #015404: Broderius, Steven J., Kahl, Michael D., and Hoglund, Marilyn D. 1995. Use of joint toxic response to define the primary mode of toxic action for diverse industrial organic chemicals. Environ. Toxicol. Chem. 14(9): 1591-605.

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
- #006622: Alexander, Howard C., Bodner, Kenneth M., and Mayes, Monte A. 1983. Evaluation of the OECD Fish Prolonged Toxicity Study at Least 14 Days. Chemosphere 12(3): 415-23.
-SDO
- #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, Emanuele, Bettiol, Cinzia, Ghelli, Anna, Todeschini, Roberto, and Miana, Paola. 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
- #009344: Barrows, M. E., Petrocelli, S. R., Macek, K. J., and Carroll, J. J. 1980. Bioconcentration and elimination of selected water pollutants by the Bluegill Sunfish (*Lepomis macrochirus*). Dyn. Exposure Hazard Assess. Toxic Chem., (Pap. Symp. 1978), Ann Arbor Sci., Ann Arbor, MI:379-392.
-NUE; BCF data, only
- #V1015: Basak, S. C., Grunwald, G. D., Gute, B. D., Balasubramanian, K., and Opitz, D. 2000. Use of statistical and neural net approaches in predicting toxicity of chemicals. J Chem Inf Comput Sci 40(4): 885-90.
-QSAR / SDO
- #005990: Batte, G. and Swanson, L. E. 1952. Laboratory Evaluation of Organic Compounds as Molluscicides and Ovocides, II. J Parasitol 38: 65-68.
-NUE.
- #V1008: Bazin, C., Chambon, P., Bonnefille, M., and Larbaigt, G. 1987. Compared sensitivity of luminescent marine bacteria (*Photobacterium phosphoreum*) and *Daphnia* bioassays (Comparaison des Sensibilites du Test de Luminescence Bacterienne (*Photobacterium phosphoreum*) et du Test *Daphnie* (Dap. Sci.Eau. 6: 403-413.
-REJECT: TONS; SW
- #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, Anna P. and Schultz, T. Wayne. 1997. Structure-activity relationships for *Pimephales* and *Tetrahymena*: a mechanism of action approach. Environ. Toxicol. Chem. 16(6): 1311-1317.

-QSAR / SDO

#V2020: Beirat der Bundesärztekammer. 1989. Belastung der Bevölkerung durch Perchlorethylen. Deutsches Rzteblatt 86, Heft 49: C2239-C2241.

-NUE

#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

#014954: Bitton, G., Rhodes, K., Koopman, B., and Cornejo, M. 1995. Short-term toxicity assay based on daphnid feeding behavior. Water Environ. Res. 67(3): 290-293.

-IITM/C data are at least partially duplicated in Ref #016609

#V2032: Black, Marsha C., Bjorkroth, Katri, and Oikari, Aimo. 1995. Probing the routes, rates, and mechanisms of xenobiotic elimination by Rainbow Trout (*Oncorhynchus mykiss*) with a physiological chamber. ASTM Spec. Tech. Publ. STP 1218(Environmental Toxicology and Risk Assessment: 3rd Vol.): 351-64.

-NUE; BCF / UDO / DEP

#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

#018325: Broderius, S. J., M. D. Kahl, G. E. Elonen, D. E. Hammermeister, and M. D. Hoglund. 2005. A comparison of the lethal and sublethal toxicity of organic chemical mixtures to the Fathead Minnow (*Pimephales promelas*). Environmental Toxicology and Chemistry 24(12): 3117-27.

-SDO.

#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.

-REJECT (TM/CU; IITM/C: low D.O. in undetermined test runs; also, solubility problems coupled with unmeasured concentrations in some tests).

#RA 1199 .E5 77-066: Carlson, R. M. and Caple, R. 1977. Chemical/biological implications of using chlorine and ozone for disinfection. Epa-600/3-77-066, U.S.Epa, Duluth, Mn:88 P.(U.S.Ntis Pb-270694) .

-SDO.

#015455: Carlson, R. M., Kopperman, H. L., Caple, R., and Carlson, R. E. 1975. Structure-activity relationships applied. Int.Joint Comm.Symp.Structure-Activity Correlations in Studies of Toxicity and Bioconcentration with Aquatic Organisms, March 11-13, 1975, Canada Center for Inland Waters, Burlington, Ontario, Can.:57-72 .

-REJECT (methodology insufficiently described)

#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

#V1116: Cronin, Mark T. D. and Schultz, T. Wayne. 1997. Validation of *Vibrio fischeri* acute toxicity data: mechanism of action-based QSARs for non-polar narcotics and polar narcotic phenols. Sci. Total Environ. 204(1): 75-88.

-NUE; TONS; QSAR / SDO

#V1146: Curtis, Carolanne, Lima, Ann, Lozano, S. J., and Veith, G. D. 1982. Evaluation of a bacterial bioluminescence bioassay as a method for predicting acute toxicity of organic chemicals to fish. ASTM Spec. Tech. Publ. 766(Aquat. Toxicol. Hazard Assess.): 170-8.

-NUE; TONS; SDO

#A00020 011588: DeVault, D. S. 1985. Contaminants in fish from Great Lakes harbors and tributary mouths. Archives of Environmental Contamination and Toxicology 14: 587-594.

-REJECT (BCF/uptake data only, ambient data only)

#V2106: Devillers, J. and Chambon, P. 1986. Acute toxicity and QSAR of chlorophenols on *Daphnia magna*. Bull. Environ. Contam. Toxicol. 37(4): 599-605.

-QSAR / SDO; 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. Advantage of the dosage-action-time relation in ecotoxicology for the test of the various chemical species of toxics (Interet de la Relation Dose-Effet-Temps en Ecotoxicologie pour la Determination des Differentes Classe. Tech.Sci.Munic. 80(7-8): 329-334.

-NUE; TDI

#V1172: Devillers, James, Chambon, Paul, Zakarya, Driss, and Chastrette, Maurice. 1986. Quantitative structure-activity relations of lethal effects of 38 halogenated compounds on *Lepomis macrochirus*. C. R. Acad. Sci., Ser. 3 303(14): 613-16.

-NUE; QSAR / SDO

#012466: Dietz, F. and Traud, J. 1978. Odor and taste threshold concentrations of phenolic compounds. Gas-Wasserfach, Wasser - Abwasser 119(6): 318-25.

-NUE;

#V1236: Eldred, Donald V., Weikel, Cara L., Jurs, Peter C., and Kaiser, Klaus 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

#014615: Enslein, Kurt, Tuzzeo, Thomas M., Borgstedt, Harold H., Blake, Benjamin W., and Hart, Jeffrey B. 1987. Prediction of rat oral LD50 from *Daphnia magna* LC50 and chemical structure. QSAR Environ. Toxicol., Proc. Int. Workshop, 2nd Meeting Date 1986, 91-106. Editor(s): Kaiser, Klaus L. E. Publisher: Reidel, Dordrecht, Neth..

-QSAR/SDO

#V1240: Escuder-Gilabert, L., Martin-Biosca, Y., Sagrado, S., Villanueva-Camanas, R. M., and Medina-Hernandez, M. J. 2001. Biopartitioning micellar chromatography to predict ecotoxicity. Analytica Chimica Acta 448(1-2): 173-185.

-NUE; SDO

#V1237: Espinosa, G., Arenas, A., and Giralt, Francesc. 2002. An integrated SOM-Fuzzy ARTMAP Neural System for the evaluation of toxicity. Journal of Chemical Information and Computer Sciences 42(2): 343-359 .

-NUE; SDO

#V1253: Feng, Liu, Han, Shuokui, Zhao, Yuanhui, Wang, Liangsheng, and Chen, Jingwen. 1996 . Toxicity of organic chemicals to Fathead Minnow: A United Quantitative Structure-Activity Relationship Model and Its Application. Chem. Res. Toxicol. 9(3): 610-13.

-QSAR; SDO

#V1270: Fent, Karl and Hunn, Judith. 1996. Cytotoxicity of organic environmental chemicals to fish liver cells (PLHC-1). Mar. Environ. Res. 42(1-4): 377-382.

-NUE

#016600: Gao, Chao, Govind, Rakesh, and Tabak, Henry H. 1992. Application of the group contribution method for predicting the toxicity of organic chemicals. Environ. Toxicol. Chem. 11(5): 631-6.

-REJECT (IITM/C; TM/CU e.g. no controls)

#V1311: Gersdorff, W. A. and Smith, L. E. 1940. Effect of introduction of the halogens into the phenol molecule on toxicity to Goldfish. I. Monochlorophenols. Am.J.Pharm. 112: 197-204.

-NUE

#V1340: Hall, Lenwood W, Hall, W. Scott, Bushong, Steven J., and Herman, Roger L. 1987. *In situ* Striped Bass (*Morone saxatilis*) contaminant and water quality studies in the Potomac River. Aquat. Toxicol. 10(2-3): 73-99.

-ISDO

#013976: Hall, Lowell H. and Kier, Lemont B. 1984. A molecular connectivity study of phenols and their toxicity to fish. QSAR Des. Bioact. Compd. 53-9. Editor(s): Kuchar, M. Publisher: Prous, Barcelona, Spain..

-REJECT (chemical mixture testing, only; no chemical-specific testing).

#009690: Hall, Lowell H., Kier, Lemont B., and Phipps, Gary. 1984. Structure-activity relationship studies on the toxicities of benzene derivatives: I. An additivity model. Environ. Toxicol. Chem. 3(3): 355-65.

-REJECT (test duration/endpoint unuseable).

#V1342: Hoke, R A, Giesy, J P, Zabik, M, and Unger, M, 1994. Toxicity of sediments and sediment pore waters from the Grand Calumet River-Indiana Harbor, Indiana Area of Concern.

- SED

#009917: Holcombe, Gary W., Phipps, Gary L., Sulaiman, Abdul H., and Hoffman, Alex D. 1987. Simultaneous multiple species testing: acute toxicity of 13 chemicals to 12 diverse freshwater amphibian, fish, and invertebrate families. Arch. Environ. Contam. Toxicol. 16(6): 697-710.

-ND.

#V1401: Jaworska, J. S. and Schultz, T. W. 1993. Quantitative relationships of structure-activity and volume fraction for selected nonpolar and polar narcotic chemicals. SAR QSAR Environ. Res. 1(1): 3-19.
-QSAR / SDO

#V1416: Kaiser, Klaus L. E., Dixon, D. George, and Hodson, Peter V. 1984. QSAR studies on chlorophenols, chlorobenzenes and para-substituted phenols. Proc. Workshop Quant. Struct.-Act. Relat. QSAR Environ. Toxicol. 189-206.
-QSAR / SDO

#V1422: Karabunarliev, Stoyan, Mekenyan, Ovanes G., Karcher, Walter, Russom, Christine L., and Bradbury, Steven 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.
-QSAR / SDO

#V1424: Kasokat, Thomas, Nagel, Roland, and Ulrich, Klaus. 1989. Metabolism of chlorobenzene and hexachlorobenzene by the Zebra Fish, *Brachydanio rerio*. Bull. Environ. Contam. Toxicol. 42(2): 254-61.
-NUE; TONNA

#010495: Keen, R. and Bailod, C. R. 1985. Toxicity to *Daphnia* of the end products of wet oxidation of phenol and substituted phenols. Water Research 19(6): 767-772.
-TM/CU; IITM/C

#003169: Kenaga, Eugene E. 1982. Predictability of chronic toxicity from acute toxicity of chemicals in fish and aquatic invertebrates. Environ. Toxicol. Chem. 1(4): 347-58.
-SDO.

#V2804: Kim, B. C., K. S. Park, S. D. Kim, and M. B. Gu. 2003. Evaluation of a high throughput toxicity biosensor and comparison with a *Daphnia magna* bioassay. Biosensors & Bioelectronics 18(5-6): 821-6.
-SDO.

#014478: Kishino, T. and Kobayashi, K. 1995. Relation between toxicity and accumulation of chlorophenols at various pH, and their absorption mechanism in fish. Water Res. 29(2): 431-442.
-NUE

#V1470: Kishino, T. and Kobayashi, K. 1996. Studies on the mechanism of toxicity of chlorophenols found in fish through Quantitative Structure-Activity Relationships. Water Res. 30(2): 393-399.
-NUE

#V1471: Kishino, Takuo and Kobayashi, Kunio. 1996. Acute toxicity and structure-activity relationships of chlorophenols in fish. Water Research 30: 387-92.
-NUE

#015583: Knie, J., Halke, A., Juhnke, I., and Schiller, W. 1983. Results of studies on chemical substances with four biotests. (Ergebnisse Der Untersuchungen Von Chemischen Stoffen Mit Vier Biotests). Dtsch. Gewaesserkd. Mitt. 27(3): 77-79.
-REJECT (No test duration given; IITM/C)

#015583: Knie, Joachim, Haelke, Arndt, Juhnke, Ingolf, and Schiller, Wolfgang. 1983. Results of studies of chemical substances using four biotests. Dtsch. Gewaesserkd. Mitt. 27(3): 77-9.
-No test duration given; IITM/C

#005473: Kobayashi, K., Akitake, H., and Manabe, K. 1979. Relation between toxicity and accumulation of various chlorophenols in Goldfish. Bull. Jpn. Soc. Sci. Fish./Nippon Suisan Gakkaishi 45(2): 173-175.
-NUE

#000816: Koch, R. 1982. Molecular connectivity and acute toxicity of environmental pollutants. Chemosphere 11(9): 925-31.
-REJECT (theoretical discussion/SDO).

#013449: Kopperman, Herbert L., Carlson, Robert M., and Caple, Ronald. 1974. Aqueous chlorination and ozonation studies. I. Structure-toxicity correlations of phenolic compounds to *Daphnia magna*. Chem.-Biol. Interact. 9(4): 245-51.
-REJECT (test organisms fed during test; test temperature inappropriate).

#V1487: Kovacs, T. G., Martel, P. H., Voss, R. H., Wrist, P. E., and Willes, R. F. 1993. Aquatic toxicity equivalency factors for chlorinated phenolic compounds present in pulp mill effluents. Environ. Toxicol. Chem. 12(2): 281-9.
-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

#010310: Kuhn, R., Pattard, Monika, Pernak, Klaus Dieter, and Winter, Angela. 1989. Results of the harmful effects of water pollutants to *Daphnia magna* in the 21 day reproduction test. Water Res. 23(4): 501-10.
-Test concentrations measured only 2 x during test; high COD; food used was problematic

#V1523: Lammering, M. W. 1961. The toxicity of phenol, o-chlorophenol, and o-nitrophenol to Bluegill Sunfish. Proc. 15th Ind. Waste Conf., Purdue Univ. Eng. Ext. Ser. No. 106: 541-555.
-NUE

#V2332: Layiwola, P. J., Linnecar, D. F. C., and Knights, B. 1983. The biotransformation of three carbon-14 labeled phenolic compounds in twelve species of freshwater fish. Xenobiotica 13(2): 107-13.
-NUE; MET; TONNA

#013840: Leblanc, G. A. 1984. Comparative structure- toxicity relationships between acute and chronic effects to aquatic organisms. QSAR in environmental toxicology. Proc. workshop, Hamilton, Ont., 1983 : 235-260.
-REJECT (IITM/C; analysis & results questionable; no acute data so no ACR possible)

#013412: LeBlanc, Gerald A., Hilgenberg, Barbara, and Cochrane, Bruce 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)

#V1528: 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

#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

#005766: McLeese, D. W., Zitko, V., and Peterson, M. R. 1979. Structure-lethality relationships for phenols, anilines and other aromatic compounds in shrimp and clams. Chemosphere 8(2): 53-57.
-NUE; QSAR/SDO

#V1593: Miyazaki, A., Amano, T., Saito, H., and Nakano, Y. 2002. Acute toxicity of chlorophenols to earthworms using a simple paper contact method and comparison with toxicities to fresh water organisms. Chemosphere 47(1): 65-9.
-TONS OR SDO

#V1614: Nalecz-Jawecki, G. and Sawicki, J. 2002. A comparison of sensitivity of spirotox biotest with standard toxicity tests. Arch Environ Contam Toxicol 42(4): 389-95.
-TONS

#V1618: Netzeva, T. I., Aptula, A. O., Benfenati, E., Cronin, M. T., Gini, G., Lessigiarska, I., Maran, U., Vracko, M., and Schüürmann, G. 2005. Description of the electronic structure of organic chemicals using semiempirical and ab initio methods for development of toxicological QSARs. J Chem Inf Model 45(1): 106-14.
-NUE; QSAR / SDO

#V1616: Niculescu, S. P., Atkinson, A., Hammond, G., and Lewis, M. 2004. Using fragment chemistry data mining and probabilistic neural networks in screening chemicals for acute toxicity to the Fathead Minnow. SAR QSAR Environ Res 15(4): 293-309 .
-NUE; QSAR / SDO

#V1620: Nouwen, Johan , Lindgren, Fredrik, Hansen, Bjorn, and Karcher, Walter. 1996. Fast screening of large databases using clustering and PCA based on structure fragments. J. Chemom. 10(5 & 6): 385-398.
-QSAR / SDO

#013826: Oikari, A., Kukkonen, J., and Virtanen, V. 1992. Acute toxicity of chemicals to *Daphnia magna* in humic waters. Science of the Total Environment 117-118: 367-377.
-TM/CU; IITM/C

#V2801: Papa, E., Villa, F., and Gramatica, P. 2005. Statistically validated QSARs, based on theoretical descriptors, for modeling aquatic toxicity of organic chemicals in *Pimephales promelas* (Fathead Minnow). Journal of chemical information and modeling 45(5): 1256-66.
-QSAR / SDO.

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-IITM/C; or SDO

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-QSAR / SDO
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-QSAR / SDO

- #V1927: Wang, X., Dong, Y., Xu, S., Wang, L., and Han, S. 2000. Quantitative structure-activity relationships for the toxicity to the tadpole *Rana japonica* of selected phenols. Bull. Environ. Contam. Toxicol. 64(6): 859-865.
-TONNA; QSAR / SDO
- #V2807: Westbury, A.-M., M. St. J. Warne, and R. P. Lim. 2004. Toxicity of, and development of predictive models for, substituted phenols to *Ceriodaphnia* cf. *dubia* and *Vibrio fischeri*. Australasian Journal of Ecotoxicology 10(1): 33-42.
-TONNA; TONS.
- #018068: Yen, J. H., K. H. Lin, and Y. S. Wang. 2002. Acute lethal toxicity of environmental pollutants to aquatic organisms. Ecotoxicology and Environmental Safety 52(2): 113-6.
-NUE: TDI; TM/CU; IITM/C; PD.
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-QSAR / SDO.

*For abbreviations used, see Appendix.

APPENDIX: REFERENCE ABBREVIATIONS USED, 4/06

AMD = ambient monitoring data.
BCF = bioconcentration factor.
D = data (as a suffix to other abbreviations listed here).
DO = data only (as a suffix to other abbreviations listed here)..
EF = environmental fate.
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.
NUE = no useable endpoint.
O = only (as a suffix to other abbreviations listed here).
PD = phytotoxicity 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.
UD or UP = uptake data.
WET = whole-effluent testing.