

Rule 57 Aquatic Values Data Sheet

1/14/2010

Chemical or product name: 2-Nitrophenol

Manufacturer (WTAs): -----

C.A.S #: 88-75-5

Developed by: Christopher Hull

Approved by: D. Bush

Approval date: 1/28/2010

CAS: 11/19/09; AQUIRE: 11/17/09; QSAR: 12/09/09

Clearinghouse search date: 12/05/95

FAV*: 1,000 ug/l

AMV*: 510 ug/l

FCV*: 56 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	150	----	13,170	13,170	13,170	1	1
Fathead Minnow (<i>Pimephales promelas</i>)	EC50	96	FT,M	44	-----	138,000	138,000	138,000	2	2
	LC50	96	FT,M	44	-----	160,000 ¹				2

*Value rounded to 2 significant figures.

¹ Value not used to calculate SMAV, because EC50 preferred over LC50 from the same test.

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
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NO SUITABLE DATA WERE FOUND.

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: 2-Nitrophenol

CAS #: 88-75-5

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Date: 1/14/10

AQUATIC MAXIMUM VALUE CALCULATIONS

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

1. Minimum requirements met = 2 (iii, iv).

2. Minimum requirements missing for Tier I = 6 (i, ii, v, vi, vii, viii).

3. Acute Factor = 13.

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

a. FAV calculation: Tier II FAV = Lowest GMAV / Acute Factor = 13,170 ug/l / 13 = 1,013.0769 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 = Tier II FAV / 2 = 1,013.0769 ug/l / 2 = 506.53846 ug/l.

RULE 57 AQUATIC VALUES WORK SHEET-CHRONIC

Chemical Name: 2-Nitrophenol
CAS #: 88-75-5
Developed by: Christopher Hull
Date: 1/14/10

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 = $X_g(18, 18, 18) = 18$.

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

$$\text{Tier II FCV} = \text{Tier II FAV} / \text{Tier II ACR} = 1,013.0769 \text{ ug/l} / 18 = \underline{56.282051 \text{ ug/l}}$$

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 = _____ = _____ = _____.

2-NITROPHENOL REFERENCES, 1/10

References Used:

1. #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.
2. #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*) Volume IV. Ctr.for Lake Superior Environ.Stud., Volume 4, Univ.of Wisconsin-Superior, Superior, WI :355 .

References Reviewed, but Not Used:

- #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.
- #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.
- #017541: Botsford, J. L. 2002. A comparison of ecotoxicological tests. *Altern Lab Anim* 30(5): 539-50.
-TONS; TMCU; or SDO.
- #V1018: Bringmann, G. and Kuhn, R. 1959. Comparative water-toxicological investigations on bacteria, algae, and *Daphnia*. *Gesundheitsingenieur* 80(4): 115-120.
-TONS, NUE.
- #V1018: Bringmann, G. and Kuhn, R. 1959. The toxic effects of waste water on aquatic bacteria, algae, and small crustaceans. *Gesund. Ing* 80: 115-120.
-TONS, NUE.
- #V1030: Bringmann, G. and Kuhn, R. 1959. Water toxicological studies with protozoa as test organisms. *Gesund. - Ing. TR-80-0058* 80: 239-242.
-NUE.
- #005672: Bringmann, G. and Kuhn, R. 1977. Results of the damaging effect of water pollutants on *Daphnia magna* (Befunde der Schadwirkung Wassergefährdender Stoffe Gegen *Daphnia magna*). *Z. Wasser-Abwasser-Forsch* 10(5): 161-166.
-TDI.
- #V1005: Bringmann, G. and Kuhn, R. 1980. Determination of the biological effect of water pollutants in protozoa. II. Bacteriovorous ciliates (Bestimmung der Biologischen Schadwirkung Wassergefährdender Stoffe Gegen Protozoen. II. Bakterienfressende Ciliaten. *Z. Wasser-Abwasser-Forsch* 13(1): 26-31.
-NUE; TONS.
- #V1006: Bringmann, G. and Kuhn, R. 1981. Comparison of the effect of toxic substances on the flagellate organisms such as ciliates and the holozoic bacteria-devouring organisms such as saprozoic protozoans (Vergleich der Wirkung von Schadstoffen auf Flagellate). *Gwf-Wasser Abwasser* 122(7): 308-313.
-NUE; TONS.
- #005672: Bringmann, G. and Kuhn, R. 1977. Results of the damaging effect of water pollutants on *Daphnia magna*. *Z. Wasser Abwasser Forsch.* 10(5): 161-6.
-TDI.
- #011330: Bringmann, G. and Kuhn, R. 1982. Results of toxic action of water pollutants on *Daphnia magna* Straus tested by an improved standardized procedure. *Z. Wasser Abwasser Forsch.* 15(1): 1-6.
-TDI; test volume loading violate ASTM standards.
- #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.
- #V3102: Costescu, A., & M. V. Diudea. (2006). QSTR study on aquatic toxicity against *Poecilia reticulata* and *Tetrahymena pyriformis* using topological indices. Vol. 5, 116-134.

-MOD / QSAR / SDO.

#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.

#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, 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.

#014615: Enslein, K., Tuzzeo, T. M., Borgstedt, H. H., Blake, B. W. , and Hart, J. 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.

#015326: Fiedler, H., Hutzinger, O., and Giesy, J. P. 1990. Utility of the QSAR modeling system for predicting the toxicity of substances on the European inventory of existing commercial chemicals. *Toxicological and Environmental Chemistry* 28(2/3): 167-188.

-QSAR / SDO.

#005855: Gersdorff, W. A. 1939. Effect of the introduction of the nitro group into the phenol molecule on toxicity to Goldfish. *J. Cell. Comp. Physiol.* 14: 61-71.

-NUE; TTDO.

#V1340: Hall, L. W., Hall, W. S., Bushong, S. J., and Herman, R. 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.

#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.

#V1417: Kaiser, K. L. E., Niculescu, S. P., and Schuurmann, G. 1997. Feed forward back-propagation neural networks and their use in predicting the acute toxicity of chemicals to the Fathead Minnow. [Erratum to document cited in CA127:132092]. *Water Qual. Res. J. Can.* 32(4): 855.

-NUE.

#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.

#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.

-QSAR / SDO.

#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.

#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.

#018359 V2859: Lee, Y. G., S. H. Hwang, and S. D. Kim. 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.

-ITM/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.

#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.

#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.

#V2857: Pavan, M., T. I. Netzeva, and A. P. Worth. 2006. Validation of a QSAR model for acute toxicity. SAR and QSAR in Environmental Research 17(2): 147-171.
-QSAR/SDO.

#009495: Rawlings, G. D. and Samfield, M. 1979. U. S. Environ. Prot. Agency, Off. Res. Dev., [Rep.] EPA EPA-600/7-78-168, Symp. Proc. Process Meas. Environ. Assess., 1978; PB-290 331, 153-69 .
-WETO.

#015372: Saito, H., Koyasu, J., Yoshida, K., Shigeoka, T., and Koike, S. 1993. Cytotoxicity of 109 chemicals to goldfish GFS cells and relationships with 1-octanol/water partition coefficients. Chemosphere 26(5): 1015-28.
-NUE.

#V2645: Schueuermann, G., Somashekar, R. K., and Kristen, U. 1996. Structure-activity relationships for chloro- and nitrophenol toxicity in the pollen tube growth test. Environ. Toxicol. Chem. 15(10): 1702-1708.
-NUE; QSAR.

#V1797: Schultz, T. W. 1997. Tetratox: *Tetrahymena pyriformis* population growth impairment endpoint-a surrogate for fish lethality. Toxicol. Methods 7(4): 289-309.
-NUE; TONS.

#V2858: Sánchez-Bayo, F. 2006. Comparative acute toxicity of organic pollutants and reference values for crustaceans. I. Branchiopoda, Copepoda and Ostracoda. Environmental Pollution 139(3): 385-420.
-QSAR / SDO.

#V1883: Veith, G. D. and Mekenyan, O. G. 1993. A QSAR approach for estimating the aquatic toxicity of soft electrophiles QSAR for soft electrophiles. Quantitative Structure-Activity Relationships 12(4): 349-356.
-QSAR / SDO.

#V1876: Wang, G. and Bai, N. 1997. Study on QSAR for general pollutants in organic industrial waste. Toxic Subst. Mech. 16(4): 315-326.
-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.

#V2856: Wang, Y.-F. and Y.-X. Lu. 2004. Assessment of acute toxicity of 13 kinds of nitrobenzol compound by aquatic ecological toxicological assay. Journal of Xinxiang Medical College (Chinese) 21(6): 456-457.
-ND.

#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, #V2806 : Yen, J. H., Lin, K. H., and Wang, Y. S. 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.

#V1881: Yoshioka, Y., Ose, Y., and Sato, T. 1986. Correlation of the five test methods to assess chemical toxicity and relation to physical properties. *Ecotoxicol. Environ. Saf.* 12(1): 15-21.

-TONNA.

#V1882: Yoshioka, Y. and Ose, Y. 1993. A quantitative structure-activity relationship study and ecotoxicological risk quotient for the protection from chemical pollution. *Environ. Toxicol. Water Qual.* 8(1): 87-101.

-QSAR / SDO.

#014780: Zhao, Y.-H., X. Yuan, G.-D. Ji, L.-X. Sheng, and L.-S. Wang. 1997. Quantitative Structure-Activity Relationships of nitroaromatic compounds to four aquatic organisms. *Chemosphere* 34(8): 1837-1844.

-TDI; SDO; IITM/C.

* For abbreviations used, see Appendix, attached.