

Rule 57 Aquatic Values Data Sheet

1/25/2010

Chemical or product name: *Methyl ethyl ketone*
 Manufacturer (WTAs): ----
 C.A.S #: 78-93-3

Developed by: *Christopher Hull* FAV*: 40,000 ug/l (Tier: II)
 Approved by: *D. Bush* AMV*: 20,000 ug/l (Tier: II)
 Approval date: *1/28/2010* FCV*: 2,200 ug/l (Tier: II)
 CAS: 11/23/09; AQUIRE: 11/12/09; QSAR: 12/11/09 Acute CF: ---- Chronic CF: ----
 Clearinghouse search date: ----

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	----	>520,000	>520,000	>520,000	1	1
Fathead Minnow (<i>Pimephales promelas</i>)	EC50	96	FT,M	47.7	----	3,220,000 ¹	3,220,000	3,220,000	2	2
	LC50	96	FT,M	47.7	----	3,220,000 ¹				2
	LC50	96	FT,M	56.3	----	3,200,000 ¹				3
	LC50	96	FT,M	45.5	----	3,200,000 ¹				4

*Value rounded to 2 significant figures.

¹ These data are all considered to be from the same study; therefore, the EC50 was used to calculate the SMAV, since EC50 is 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
---------	--------------------------	--------------------	------------------------------------	------------------	------------------	--------------	--------------	--------------	------	-----------

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: Methyl ethyl ketone

CAS #: 78-93-3

Developed by: Christopher Hull

Date: 1/25/10

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 = $520,000 \text{ ug/l} / 13 = \underline{40,000 \text{ ug/l}}$.

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 = $\text{Tier II FAV} / 2 = 40,000 \text{ ug/l} / 2 = \underline{20,000 \text{ ug/l}}$.

RULE 57 AQUATIC VALUES WORK SHEET-CHRONIC

Chemical Name: Methyl ethyl ketone

CAS #: 78-93-3

Developed by: Christopher Hull

Date: 1/25/10

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.

Tier II FCV = Tier II FAV / Tier II ACR = $40,000 \text{ ug/l} / 18 = \underline{2,222.2222 \text{ ug/l}}$.
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 = _____ = _____ = _____.

METHYL ETHYL KETONE REFERENCES, 1/10

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. #QL 638 .C94 A27 v.1: Brooke, L. T., Call, D. J., Geiger, D. L., and Northcott, C. E., 1984. Acute toxicities of organic chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 1. Center for Lake Superior Environmental Studies, University of Wisconsin.
3. #000815: Veith, G. D., Call, D. J., and Brooke, L. T. 1983. Estimating the acute toxicity of narcotic industrial chemicals to Fathead Minnows. ASTM Spec. Tech. Publ. 802(Aquat.Toxicol.Hazard Assess.): 90-7.
4. #007358: Veith, G. D., Call, D. J., and Brooke, L. T. 1983. Structure-toxicity relationships for the Fathead Minnow, *Pimephales promelas*: narcotic industrial chemicals. Can. J. Fish. Aquat. Sci. 40(6): 743-8.

References Reviewed, but Not Used*:

- #013562: Abernethy, S. G., Mackay, D., and McCarty, L. S. 1988. Volume fraction correlation for narcosis in aquatic organisms: the key role of partitioning. Environ. Toxicol. Chem. 7(6): 469-81.
-SDO.
- #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.
- #V1004: Brandao, J. C., Bohets, H. H. L., Van de Vyver, I. E., and Dierickx, P. J. 1992. Correlation between the in vitro cytotoxicity to cultured Fathead Minnow fish cells and fish lethality data for 50 chemicals. Chemosphere 25(4): 553-62.
-NUE; TONS.
- #V1006: Bringmann, G. and R. Kuhn. 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.
- #V1005: Bringmann, G. and R. Kuhn. 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.
-REJECT: No useable endpoint: Test organisms not suitable.
- #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.
-REJECT: (test duration inappropriate).
- #011330: Bringmann, G. and R. Kuhn. 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.
- #V1021: Buzzell, J. C. J., Young, R. H. F., and Ryckman, D. W., 1968. Behavior of organic chemicals in the aquatic environment. Part II. - Behavior in dilute systems. Environ Sanitary Engineering Labs, Washington University.
-NUE.
- #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.
- #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.
- #V1146: Curtis, C., Lima, A., 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.
- #V1208: Devillers, J., Elmouaffek, A., Zakarya, D., and Chastrette, M. 1987. Comparison of ecotoxicological data

by means of an approach combining cluster and correspondence factor analyses. *Chemosphere* 17(4): 633-46.
-NUE; TONS.

#V2112: Dierickx, P. J. 1993. Correlation between the reduction of protein content in cultured FHM fish cells and fish lethality data. *Toxicology in Vitro* 7(4): 527-530.
-NUE; SDO.

#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.

#V1237: Espinosa, G., Arenas, A., and Giralt, F. 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

#016600: Gao, C., Govind, R., and Tabak, H. 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).

#V3097: Hahin, R., Larsen, J., and Gasser, K. 2008-. Predictions of the EC50 for action potential block for aliphatic solutes. *Journal of Membrane Biology* 221(2): 73-85.
-NUE: MOD, SDO.

#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.

#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.
-ACCEPT only for ACR calculation (SW), if suitable chronic data from #007902 or other studies by this lab can be found.

#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.

#V1414: Jensen, R. A., 1978. A simplified bioassay using finfish for estimating potential spill damage .
- NUE.

#008079: Juhnke, I. and D. Luedemann. 1978. Results of the investigation of 200 chemical compounds for acute fish toxicity with the Golden Orfe Test (Ergebnisse der Untersuchung von 200 Chemischen Verbindungen auf Akute Fischtoxizität mit dem Goldorfe Test). *Z. Wasser-Abwasser-Forsch.* 11(5): 161-164.
-SDO; TONNA; TDI. Methods for this study are in Mann (1976), attached to this paper under the same library number.

#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.

#V2266: Kamlet, M J, Doherty, R M, Veith, G D, Taft, R W, and Abraham, M H, 1987. Solubility properties in polymers and biological media. 7. An analysis of toxicant properties that influence inhibition of bioluminescence in '*Photobacterium phosphoreum*' (The Microtox Test).
- TONS; NUE.

#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.
-NUE.

#010251: Kramer, V. C., Schnell, D. J., and Nickerson, K. W. 1983. Relative toxicity of organic solvents to *aedes aegypti* Larvae. *Journal of Invertebrate Pathology* 42: 285-287.

-TDI

#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.

#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.

#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.

#015384: Nishiuchi, Y. 1981. Toxicity of pesticides to some aquatic animals. II. Toxicity of several solvents to carp and *Daphnia*. Seitai Kagaku 4(3): 45-7.

-TDI.

#V2507: Noever, D. A., Matsos, H. C., Cronise, R. J., Looger, L. L., Relwani, R. A., and Johnson, J. U. 1994. Computerized *in vitro* test for chemical toxicity based on *Tetrahymena* swimming patterns. Chemosphere 29(6): 1373-1384.

-TONS.

#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.

#015353: Protic, M. and Sabljic, A. 1989. Quantitative structure-activity relationships of acute toxicity of commercial chemicals on fathead minnows: effect of molecular size. Aquatic Toxicology 14(1): 47-64.

-QSAR/SDO.

NIL: Raevsky, O. A., Grigor'ev, V. Y., Weber, E. E., and Dearden, J. C. 2008. Classification and Quantification of the Toxicity of Chemicals to Guppy, Fathead Minnow and Rainbow Trout: Part I. Nonpolar Narcosis Mode of Action. QSAR & Combinatorial Science 27(11-12): 1274-1281.

#015771: Ramos, E. U., Vaes, W. H. J., Verhaar, H. J. M., and Hermens, J. L. M. 1998. Quantitative Structure-Activity Relationships for the aquatic toxicity of polar and nonpolar narcotic pollutants. Journal of Chemical Information and Computer Sciences 38(5): 845-852.

-QSAR/SDO.

#007715: Randall, T. L. and Knopp, P. V. 1980. Detoxification of specific organic substances by wet oxidation. J Water Pollut Control Fed 52(8): 2117-2130.

-IITM/C; or SDO.

#V2826: Robinson, P. W. 1999. The toxicity of pesticides and organics to Mysid Shrimps can be predicted from *Daphnia* spp. toxicity data. Water Research 33(6): 1545-1549.

-SD; SW.

#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.

#V2649: Schultz, T. W., Sinks, G. D., and Hunter, R. S. 1995. Structure-Toxicity Relationships for alkanones and alkenones. SAR and QSAR in Environ. Res. 3: 27-36.

-TONS.

#V1748: Sixt, Stefan and Altschuh, Joachim, 1997. Prediction of luminescent bacteria toxicity using quantum

chemical descriptors: test of a classification scheme. Quantitative Structure-Activity Relationships in Environmental Sciences-VII, Proceedings of QSAR 96, Elsinore, Den., June 24-28, 1996.

- QSAR; SD; 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.

#015390: Tanaka, A., Masago, H., Kanou, K., and Ujiie, A. 1984. Studies on the simplified assay for the trace amounts of agricultural chemicals in water and its acute toxicity to fishes. (3). 2. Simplified and rapid assay for organophosphorus pesticides and the acute toxicity to the tropical fish, guppy. Yosui to Haisui 26(5): 529-37.

-TDI.

#008617: Turnbull, H. , Demann, J. G., and Weston, R. F. 1954. Toxicity of various refinery materials to fresh water fish. Ind.Eng.Chem. 46(2): 324-333.

-NUE; TDI.

#015355: Vaishnav, D. D. and Korthals, E. T. 1990. Comparative toxicities of selected industrial chemicals to microorganisms and other aquatic organisms. Arch. Environ. Contam. Toxicol. 19(4): 624-8.

-SDO.

#010999: Vaishnav, D. D. 1986. Chemical structure-biodegradation inhibition and fish acute toxicity relationships for narcotic industrial chemicals. Toxic. Assess. 1(2): 227-40.

-SDO.

#004260: Wallen, I. E., Greer, W. C., and Lasater, R. 1957. Toxicity to *Gambusia affinis* of certain pure chemicals in turbid waters. Sewage Ind. Wastes 29(6): 695-711.

-REJECT (TM/CU: test water highly turbid, and aerated).

*For abbreviations used, see Appendix, attached.

APPENDIX: REFERENCE ABBREVIATIONS USED, 1/10

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.
GWD = groundwater data.
ITM/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.