Chemical or product name: Nitrobenzene

Manufacturer (WTAs): 
C.A.S #: 98-95-3

Developed by: Christopher Hull  
FAV*: 2,100 ug/l

Approved by: D. Bush  
AMV*: 1,000 ug/l

Approval date: 2/8/2010  
FCV*: 230 ug/l

CAS, AQUIRE: 11/25/09; QSAR: 12/11/09

Clearinghouse search date: 6/13/96

Acute CF: 
Chronic CF: ----

### ACUTE DATA

<table>
<thead>
<tr>
<th>Species</th>
<th>Endpoint</th>
<th>Duration</th>
<th>Test Type</th>
<th>Hardness</th>
<th>Test</th>
<th>LC50/EC50</th>
<th>SMAV</th>
<th>GMAV</th>
<th>Rank</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Flea (Daphnia magna)</td>
<td>LC50</td>
<td>48</td>
<td>S,U</td>
<td>173</td>
<td>------</td>
<td>27,000</td>
<td>27,000</td>
<td>27,000</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Fathead Minnow (Pimephales promelas)</td>
<td>LC50</td>
<td>96</td>
<td>FT,M</td>
<td>44.1</td>
<td>------</td>
<td>119,000</td>
<td>117,996</td>
<td>117,996</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>LC50</td>
<td>96</td>
<td>FT,M</td>
<td>44.9</td>
<td>------</td>
<td>117,000</td>
<td></td>
<td></td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>Species</td>
<td>Test type</td>
<td>Duration (days)</td>
<td>Study Conditions (FT,M etc.)</td>
<td>Hardness mg/L</td>
<td>Test Chemical</td>
<td>MATC ug/L</td>
<td>SMCV ug/L</td>
<td>GMCV ug/L</td>
<td>Rank</td>
<td>Reference</td>
</tr>
<tr>
<td>------------------------</td>
<td>-----------</td>
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<td>-----------------------------</td>
<td>---------------</td>
<td>---------------</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
<td>------</td>
<td>-----------</td>
</tr>
<tr>
<td>Fathead Minnow</td>
<td>LSG</td>
<td>7</td>
<td>FT,M</td>
<td>45.5</td>
<td>-----</td>
<td>48,375 1</td>
<td>48,375</td>
<td>48,375</td>
<td>1</td>
<td>4</td>
</tr>
</tbody>
</table>

*(Pimephales promelas)*

*Value rounded to 2 significant figures.

1 For MATC and ACR calculations, see Table 1.
Table 1. Nitrobenzene MATC and ACR calculations for Fathead Minnow from References #3 and 4*, 2/04/10 (Hull).

Acute data (Ref. #3):
96-hr. LC50 = 117,000 ug/l.

Chronic Data (Ref. #4):
7-d LSG NOECgrowth = <10,200 ug/l; LOECgrowth = <10,200 ug/l; MATCgrowth = Xg = <10,200 ug/l.
7-d LSG NOECsurvival = 38,300 ug/l; LOECsurvival = 61,100 ug/l; MATCsurvival = Xg = 48,375 ug/l.
ACR = 96-hr. LC50 / 7-d MATCsurvival = 117,000 ug/l / 48,375 ug/l = 2.4186047.

*Acute and chronic tests were conducted in different studies, by different investigators, but at the same lab (USEPA-ERL-Duluth). Both used Lake Superior water as diluent. Test organisms for acute tests were from in-house (USEPA-ERL-Duluth) cultures. Test organisms for chronic tests were from USEPA-Newtown, OH.
RULE 57 AQUATIC VALUES WORK SHEET-ACUTE

Chemical Name: Nitrobenzene
CAS #: 98-95-3
Developed by: Christopher Hull
Date: 2/04/10

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).
   4. Toxicity is not dependent upon a water quality characteristic: Yes.
      a. FAV calculation: Tier II FAV = Lowest GMAV / Acute Factor = 27,000 ug/l / 13 = \(2,076.9231 \text{ ug/l}\).
   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 = ____ (____).
         In of final acute intercept = ____.
      d. FAV equation: Tier I FAV = ____ = ____ = ____.

C. Aquatic Maximum Value (AMV) calculation: Tier II AMV = Tier II FAV / 2 = 2,076.9231 ug/l / 2 = \(1,038.4615 \text{ ug/l}\).

9/25/2007
**RULE 57 AQUATIC VALUES WORK SHEET - CHRONIC**

**Chemical Name:** Nitrobenzene  
**CAS #:** 98-95-3  
**Developed by:** Christopher Hull  
**Date:** 2/04/10

**FINAL CHRONIC VALUE CALCULATIONS**

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

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

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

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 = 1 (Table 1).
   b. Tier II Acute-to-Chronic Ratio = Xg(Table 1 ACR (FHM), 18, 18) = Xg(2.418604, 18, 18) = 9.2194136.

2. Toxicity is not dependent upon a water quality characteristic: **Yes**.
   Tier II FCV = Tier II FAV / Tier II ACR = 2.076.9231 ug/l / 9.2194136 = **225.27714** 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 = _____ = _____ = _____.

9/25/2007
NITROBENZENE REFERENCES, 2/10

References Used:

References Reviewed, but Not Used*:
-SDO.
-SDO.
-NUE; TM/CU; MDO).
-QSAR / SDO.
-QSAR / SDO.
-NUE; SDO.
-TONS, NUE.
#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.
-REJECT: No useable endpoint: Test organisms not suitable.
-REJECT: (test duration inappropriate).
#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
-NUE
-TDI
-TDI; test volume loading violate ASTM standards
-REJECT (low D.O. in undetermined test runs; also, solubility problems coupled with unmeasured concentrations in some tests)
-REJECT (insufficient information on test methodology/conditions).
-IITM/C
-REJECT (all data are either secondary, or insufficiently described).
-QSAR/SDO.
-NA; FLO.
-QSAR / SDO.
-QSAR / SDO.
-QSAR / SDO.
-QSAR / SDO.
-NUE; TONS.
-NUE; SD.
-QSAR / SDO.
Grundlage für die Bewertung der Umweltgefährlichkeit in Aquatischen Systemen. Forschungsbericht.

-NUF.


-TCM/CU.


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


-NUF.


-REJECT (test animals fed during test).


-REJECT (*C. dubia*: TDI; *FHM*: fed test; *D. magna*: SDO).


-NUF; QSAR / SDO.


-NUF; QSAR / SDO.


-NUF; QSAR / SDO.


-TDI.


-QSAR/SDO.


-QSAR/SDO.


-QSAR/SDO.


-QSAR / SDO; NA; FLO.


-MOD / QSAR / SDO.


-IITM/C especially regarding D.O. and controls; *Daphnia magna* test also violated ASTM loading standards; guppy
and snail tests had D.O. problems; snail species may not have been North American.


-SDO.


-QSAR/SDO.


-QSAR / SDO.


-SD; SW.


-NA.


-QSAR / SDO.


-TONS; NUE.


-NUE; TONS.


-QSAR / ND (on this chemical).


-TONS; NUE.


-TONS; NUE.


-NUE; SDO.


-NUE; TONNA; SD.


-QSAR / SDO.


-NUE; TDI.


-TONS.


-TONNA.


-QSAR / SDO.


-NUE.

#015458: Vander Schalie, W. H., 1983. Acute and chronic toxicity of 3,5-dinitroaniline, 1,3-dinitrobenzene, and 1,3,5-trinitrobenzene to freshwater aquatic organisms.

- Not reviewed.


-QSAR ISDO.


-NUE.

#015458: Vander Schalie, W. H., 1983. Acute and chronic toxicity of 3,5-dinitroaniline, 1,3-dinitrobenzene, and 1,3,5-trinitrobenzene to freshwater aquatic organisms.

- Not reviewed.


-QSAR ISDO.


-NUE; MOD.


-IITM/C; TM/CU; Good SRM study but no info on solvent controls. Could use for Tier III.


-SW; UDO; TATO.


-ND.


-TM/CU; IITM/C.


-MOD / QSAR / SDO.


-MOD / QSAR / SDO.


-QSAR; SDO; TONNA.


-NUE; TDI; TM/CU; IITM/C; PD.


-TONNA.


-TONS.


-QSAR / SDO.

structure-activity models developed to estimate toxicity to freshwater fish. Aquat. Toxicol. 6(4): 251-70.
- QSAR / SDO; SW.

- MOD / QSAR / SDO.

- MOD / QSAR / SDO.

- TDI; SDO; IITM/C.

- TONNA.

*For abbreviations used, see Appendix, attached.*
APPENDIX: REFERENCE ABBREVIATIONS USED, 2/10

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.