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Calculator: James Schmidt (updated due to variable responses within species)

SECONDARY VALUES FOR 4-NITROPHENOL (CAS No. 100-02-7)

A search was conducted for information on the chemical properties and toxicity of 4-nitrophenol (a.k.a. p-nitrophenol) to human health and to fish and aquatic life using the following databases and search engines: ECOTOX (toxicity to fish and aquatic life), IRIS (Integrated Risk Information System; toxicity to human health), and CHEMFATE (environmental fate).

FISH AND AQUATIC LIFE

To derive an acute toxicity criterion for aquatic life, acute toxicity test results are required for at least one species in each of eight different families. Specific requirements and the data available to meet these requirements are found in Table 1. Following a search for information on the toxicity of 4-nitrophenol to fish and other aquatic life, it was determined that data are available to meet six out of the eight requirements. Because data are available for a Daphnid species, it was possible to calculate a secondary acute value for this substance.

Cold Water

To calculate a secondary acute value (SAV), the lowest genus mean acute value (GMAV) in the database is divided by the secondary acute factor (SAF; an adjustment factor corresponding to the number of satisfied requirements).

SAF for six out of eight requirements met = 5.2

Lowest GMAV = 4,322 µg/L (*Onchonrhynchus mykiss*)

$$\begin{aligned}\mathbf{SAV} &= \mathbf{GMAV/SAF} \\ &= 4,322 \mu\text{g/L} / 5.2 \\ &= \mathbf{831.2 \mu\text{g/L}}\end{aligned}$$

SACR (secondary acute-chronic ratio) = Geometric mean of three species mean acute-chronic ratios (SMACRs). Default = 18

$$\begin{aligned}\mathbf{SCV} &= \mathbf{SAV/SACR} \\ &= 831.2 \mu\text{g/L} / 18 \\ &= \mathbf{46.2 \mu\text{g/L}}\end{aligned}$$

Because the lowest acute value was for a coldwater fish, and the next lowest was for an invertebrate, secondary values will be calculated for the non-coldwater use designations.

$$\begin{aligned}\mathbf{SAV} &= \mathbf{GMAV/SAF} \\ &= 5,171 \mu\text{g/L} / 5.2 \\ &= \mathbf{994.4 \mu\text{g/L (for warmwater sport fish, limited forage fish, limited aquatic life uses)}}\end{aligned}$$

SACR (secondary acute-chronic ratio) = Geometric mean of three species mean acute-chronic ratios (SMACRs). Default = 18

SCV = SAV/SACR
= 994.4 µg/L / 18
= **55.2 µg/L (for warmwater sport fish, limited forage fish, limited aquatic life uses)**

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for 4-nitrophenol, and corresponding acute toxicity data.

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference # ^a	Source
1. At least one salmonid fish in the family Salmonidae, in the class Osteichthyes.					
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	7,900	1	ECOTOX
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	3,800	2	ECOTOX
# <i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	78,900	2	ECOTOX
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	4,820	2	ECOTOX
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	7,070	2	ECOTOX
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	13,000	3	ECOTOX
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	4,500	3	ECOTOX
# The LC50s varied by more than a factor of 10, and since the other results were towards the lower end of the range, the high value was dropped out.					
Species Mean Acute Value (SMAV) = 4,322					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
<i>Italurus punctatus</i>	channel catfish	96-h/LC50	15,000	4	ECOTOX
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	8,300	5	ECOTOX
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	22,000	4	ECOTOX
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	6,600	4	ECOTOX
SMAV = 10,642					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
<i>Daphnia magna</i>	water flea	48-h/EC50	22,000	6	ECOTOX
<i>Daphnia magna</i>	water flea	48-h/EC50	8,400	7	ECOTOX
<i>Daphnia magna</i>	water flea	48-h/EC50	7,680	8	ECOTOX
<i>Daphnia magna</i>	water flea	48-h/EC50	4,700	9	ECOTOX

<i>Daphnia magna</i>	water flea	48-h/EC50	36,000	3	ECOTOX
<i>Daphnia magna</i>	water flea	48-h/EC50	6,000	3	ECOTOX
SMAV = 10,628					

4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).
***Gammarus pseudolimnaeus* amphipod** 96-h/LC50 2,800 2 ECOTOX
***Gammarus pseudolimnaeus* amphipod** 96-h/LC50 42,500 2 ECOTOX
*Gammarus pseudolimnaeus*. amphipod 96-h/LC50 7,540 2 ECOTOX
***Gammarus pseudolimnaeus* amphipod** 96-h/LC50 6,550 2 ECOTOX
The LC50s varied by more than a factor of 10, and since the two middle results were towards the lower end of the range, the high value was dropped out.
SMAV = 5,171
5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).
6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.
Pimephales promelas fathead minnow 96-h/LC50 59,000 11 ECOTOX
Pimephales promelas fathead minnow 96-h/LC50 62,000 11 ECOTOX
Pimephales promelas fathead minnow 96-h/LC50 41,000 4 ECOTOX
Pimephales promelas fathead minnow 96-h/LC50 37,300 12 ECOTOX
Pimephales promelas fathead minnow 96-h/LC50 41,000 12 ECOTOX
Pimephales promelas fathead minnow 96-h/LC50 58,600 12 ECOTOX
Pimephales promelas fathead minnow 96-h/LC50 33,800 13 ECOTOX
Pimephales promelas fathead minnow 96-h/LC50 30,400 13 ECOTOX
SMAV = 43,906
7. At least one organism from a family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).
Elminia livescens river snail 96-h/LC50 13,200 10 ECOTOX
8. At least one organism from a family in any order of insect or any other phylum not already represented in subdivisions 1 through 7.

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HUMAN HEALTH

To calculate a criteria or secondary value for the protection of human health, it is first necessary to determine if the substance has been shown to be carcinogenic (which will result in the calculation of a human cancer criteria or secondary value) or not (which will result in the calculation of a human threshold criteria or secondary value). 4-Nitrophenol is listed in EPA's IRIS database, but neither an oral reference dose (oral RfD) nor an oral slope factor are available. Therefore, it is not possible to calculate human threshold or cancer secondary values for this substance.