ECOTOXICITY PROFILE

23-MAR-89

U.S. Environmental Protection Agency
Environmental Research Laboratory-Duluth

I. Chemical Identification

Name Phenol, 4-nonyl-

CAS number 104-40-5
Formula C15 H24 0

II. Chemical and Physical Properties from QSAR

(All temperature sensitive values assume 25 C)

Molecular Weight (g/mole)	=	220.4	Calc.
Melting Point (C)	=	not available for this chemical	
Boiling Point (C)	=	311.	Calc.
Vapor Pressure (mm of Hg)	=	8.04E-05	Calc.
Ht Vaporization (cal/mole)	=	1.48E+04	Calc.
Solubility in Water (mg/L)	=	2.07E-02	Calc.
Log P	=	6.36	CLogP
pKa	=	9.92	Calc.

III. Information from QSAR concerning Exposure and Fate

Log(BCF)	=	4.62	See Veith and Kosian 1983
Bioconcentration Factor	=	4.18E+04	

Absorption Coef. Log(Koc)	=	4.79	See Lyman et al. 1982
Hydrolysis Half-Life	>	1000 days	

Hydrolysis is not likely to be an important
transformation mechanism for this chemical

The water solubility for this chemical is too low
for reliable estimates using Henry's constant

Mackay Level 1 Environmental Partitioning @25 C Fugacity = 4.199E-06 Pa

10.16 % into air
46.28 % into soil
0.26 % into water
0.07 % into suspended solids
0.03 % into aquatic biota
43.20 % into sediment

Biodegradation Half-life Analysis

***** QSAR OPENED SUBFILE 2 FOR AROMATIC CHEMICALS *****
EVALUATIONS OF DEGRADATION WITHIN THIS SUBFILE WERE BASED ON 86 OR ABOUT 32 % OF THE CHEMICALS IN THE DATA BASE.

LOGP WAS MORE THAN 2.18
THIS CHEMICAL IS GROUPED WITH 10 AROMATIC CHEMICALS THAT CONTAIN ONLY CARBON, OXYGEN, NITROGEN, AND HYDROGEN. QSAR DID NOT FIND ANY FUNCTIONAL GROUPS THAT APPEAR TO PROHIBIT DEGRADATION. THE RANGE OF HALF-LIFE VALUES FOR CHEMICALS IN THIS GROUP ARE BETWEEN 3 AND 17 DAYS.

IV. Toxicological Information from QSAR

Toxicity to the fathead minnow

LC50 (mg/L)	= 0.197	Calc.
MATC (mg/L)	= 9.87E-03	

Phytotoxicity Assessment

The rules for distinguishing substructures which may have inhibitory effects on plant growth and development are being formulated by Dr. Fumihiko Hayashi of the Office of Toxic Substances, Washington, D.C. HERD/EEB Room E431 Phone (202)382-4278.

This chemical does not contain structural features which the QSAR SYSTEM now regards as highly toxic to algae or aquatic plants.

Genetic/Mutagenic Assessment

There is no information in the QSAR SYSTEM which would suggest that this chemical is a potential carcinogen or mutagen.

WORKING DRAFT
2/28/89

Ambient Water Quality Advisories For

NONYLPHENOL[1]

(Chemical Abstracts Service Registry No. 25154-52-3)

Prepared by
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Prepared for
U.S. Environmental Protection Agency
Criteria and Standards Division
Office of Water Regulations and Standards
Washington, D.C.

Through
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Bioenvironmental Science Section
Columbus, Ohio 43201
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Work Assignment No. 1-25

[1] This document has been prepared according to the "Guidelines for deriving ambient aquatic life advisory concentrations" of May 1987. These "Guidelines" are being reviewed and the format and data contained in this document must be considered provisional contingent upon the outcome of peer review.

NOTICES

This document has been reviewed by the Criteria and Standards Division, Office of Water Regulations and Standards, U.S. Environmental Protection Agency, and approved for distribution.

Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

This document is available to the public through the Criteria and Standards Division, Office of Water Regulations and Standards, U.S. EPA, Washington, DC.

FOREWORD

The Criteria and Standards Division of the Office of Water Regulations and Standards has instituted water quality advisories as a vehicle for transmitting the best available scientific information concerning the aquatic life and human health effects of selected chemicals in surface waters. Advisories are prepared for chemicals for which information is needed quickly, but for which sufficient data, resources, or time are not available to allow derivation of national ambient water quality criteria.

Data supporting advisories are usually not as extensive as required for derivation of national ambient water quality criteria, and the strength of an advisory will depend upon the source, type, and reliability of the data available. We feel, however, that it is in the best interest of all concerned to make the enclosed information available to those who need it.

Users of advisories should take into account the basis for their derivation and their intended uses. Anyone who has additional information that will supplement or substantially change an advisory is requested to make the information known to us. An advisory for an individual chemical will be revised if any significant and valid new data make it necessary.

We invite comments to help improve this product.

Edmund M. Notzon, Director
Criteria and Standards Division

ACKNOWLEDGMENTS

AQUATIC LIFE

Larry T. Brooke, author
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HUMAN HEALTH

Office of Drinking Water, U.S. EPA

CONTENTS

SECTION I. EXECUTIVE SUMMAY

AQUATIC LIFE - Provisional Advisory[a]

If the estimated or measured ambient concentration of nonylphenol exceeds 0.540 µg/L in fresh or salt water, one or more of the following options must be completed within a reasonable period of time:

1. Obtain more measurements of the concentration.
2. Improve the estimate of the concentration.
3. Reduce the concentration.
4. Obtain additional laboratory and/or field data on the effect of nonylphenol on aquatic life so that a new aquatic life advisory or water quality criterion can be derived.

After a reasonable period of time, unless a consideration of all the available data concerning the ambient concentration and the effects of nonylphenol on aquatic life indicates that the ambient concentration is low enough, it must be reduced.

[a] See text for details.

SECTION III. GENERAL INFORMATION

A. Biological, Chemical, and Physical Properties

The following information on the properties of nonylphenol and its persistence in the aquatic environment was obtained from the Handbook of Chemistry and Physics[a] or from the QSAR system[b] on February 21, 1989. Some of the values were calculated using structure-activity relationships. Nonylphenol is the name for a group of chemicals having the general formula $C_{15}H_{24}O$. The nine carbon chain is usually attached to the phenol ring in the para position and can be straight or branched. Data presented in the table are the range of values for some compounds.

Property	Value	Source
Molecular Weight	220.4 g/mole	Calculated
Relative Density	0.950	Measured
Log P	6.23-6.36	Calculated
Melting Point	not available	-
Boiling Point	3.11°C	Calculated
Vapor Pressure	8.04×10^{-5}	Calculated
Heat of Vaporization	14,800 cal/mole	Calculated
pKa	9.92	Calculated
Solubility in Water	0.0207-0.0299 mg/L	Calculated
BCF	33,000-41,800	Calculated
Log BCF	4.52-4.62	Calculated
Absorption Coef.[Log (Koc)]	4.72-4.79	Calculated

Hydrolysis Half-life = >1000 days
Hydrolysis is not likely to be an important transformation mechanism for this group of chemicals.

Biodegradation Half-life Analysis
This group of chemicals would be expected to have a biodegradation half-life ranging from 3 to 17 days, based upon similar chemicals in the database.

Log 10 (Henry's Constant) = The water solubility for this group of chemicals is too low for reliable estimates using Henry's constant.

a Handbook of Chemistry and Physics, 67th Ed., CRC Press, Boca Raton, FL. 1986-1987.

b For information on the QSAR system, see: Hunter, R., L. Faulkner, F. Culver and J. Hill. Draft user manual for the QSAR system. Center for Data Systems and Analysis, Montana State University. November, 1985.

Mackay Level 1 Environmental Partitioning at 25°C
Fugacity = 3.943×10^{-6} - 4.199×10^{-6} Pa

Air	=	9.54-10.16%
Water	=	0.26-0.35%
Soil	=	46.28-46.56%
Sediment	=	43.20-43.45%
Suspended solids	=	0.07%
Aquatic biota	=	0.03%

SECTION IV. AQUATIC TOXICITY

Introduction

Aquatic life advisory concentrations are conceptually different from national aquatic life water quality criteria. Aquatic life criteria are based on toxicity and bioconcentration data for a sufficiently diverse group of animals and plants to provide reasonable confidence in the appropriateness of the criteria. Advisories are issued for selected chemicals for which sufficient data are not available to allow derivation of national water quality criteria for aquatic life. Because aquatic life advisories are intended to be used to identify situations where there is cause for concern and where appropriate action should be taken, the advisory concentration for a chemical is derived to be equal to or lower than what the Criterion Continuous Concentration (Stephan et al. 1985) would be if a national water quality criterion for aquatic life could be derived for the chemical. If the concentration of a chemical in a variety of surface waters is found to exceed the aquatic life advisory concentration, this may indicate that the U.S. EPA should consider deriving aquatic life water quality criteria for that chemical.

The literature searching and data evaluation procedures used in the derivation of aquatic life advisories are identical to those used in the derivation of water quality criteria for aquatic life (Stephan et al. 1985). However, advisories do not contain a section on "Unused Data" as in a criteria document. This aquatic life advisory concentration for nonylphenol was derived using the procedures described in the "Guidelines for Deriving Ambient Aquatic Life Advisory Concentrations" (U.S. EPA 1987). A knowledge of these guidelines is necessary in order to understand the following text, tables, and calculations. The latest comprehensive literature search for information for this aquatic life advisory was conducted in July, 1988.

Nonylphenol represents a group of chemicals having nine carbons attached to the phenol ring structure. The nine carbons can be in a straight chain or branched. The usual position for the carbon chain is in the para position.

The physical and chemical properties of nonylphenol compounds suggest that it is quite volatile and its concentration in static exposures may decline rapidly (Section III A). Based on nominal concentrations, McLeese et al. (1980b) reported a 96-hr LC50 of 900 µg/L for Atlantic salmon tested in a static exposure. In flow-through, measured exposures, they calculated 96-hr LC50s of 130 and 160 µg/L for the same species. This indicates that data from static, unmeasured exposures are likely to underestimate the toxicity of nonylphenol to aquatic organisms.

According to the advisory guidelines, data from such static exposures should be multiplied by a factor obtained by dividing a flow-through 96-hr LC50 by a comparable 96-hr LC50 derived from a static test that was measured at 0 hr. At the present time, data are not available to allow the calculation of this adjustment factor. Therefore, toxicity data derived from static, unmeasured tests could not be adjusted, and their use in the derivation of an aquatic life advisory concentration may lead to an underestimation of the actual toxicity of nonlyphenol.

Effects on Freshwater Organisms

Data on the acute toxicity of nonylphenol to freshwater animals are available for one species of fish (Table 1). In flow-through, measured exposures, the fathead minnow, Pimephales promelas, had a 96-hr LC50 of 135 µg/L (Holcombe et al. 1984; Geiger et al. 1985).

No data are available on the chronic toxicity or bioconcentration of nonylphenol in freshwater organisms.

Data are available describing other lethal and sublethal effects of nonylphenol on freshwater organisms (Table 3). The clam, Anadonta cataractae, was the most tolerant organism with a 144-hr LC50 of 1,700 µg/L (McLeese et al. 1980b). Two fish species were tested, and the fathead minnow had loss of equilibrium after a 96-hr exposure to 98 µg/L (Holcombe et al. 1984). The medaka, Orizias latipes, which is not a native species of North America, had a 48-hr LC50 of 4.36 µg/L (Yoshioka et al. 1986), which is the most sensitive response to nonylphenol reported in the literature.

Effects on Saltwater Organisms

Data on the acute toxicity of nonylphenol to saltwater organisms are available for two invertebrates and a fish tested under renewal or flow-through, measured exposure conditions (Table 1). The 96-hr LC50s for the shrimp, Crangon septemspinosa, were identical at 300 µg/L for two tests conducted by McLeese et al. (1980b, 1981). There was no difference between the technical nonylphenol and an unspecified better grade of the compound. The American lobster, Homarus americanus, had a 96-hr LC50 of 170 µg/L and was about as sensitive as the shrimp. Atlantic salmon, Salmo salar, were tested in four separate tests. Three tests had measured concentrations of nonylphenol, two of which were flow-through and the other a renewal test. The range of LC50s was from 130 to 190 µg/L. Only the flow-through tests were used to compute the Species Mean Acute Value of 144.2 µg/L, as recommended in the Guidelines (Stephan et al. 1985). A fourth test was conducted with the Atlantic salmon which was a concentration renewal and unmeasured test. The 96-hr LC50 was 900 µg/L. The much higher value in the unmeasured test than in the three measured tests is likely due to the loss of compound due to volatilization.

No data are available on the chronic toxicity of nonylphenol to saltwater animals.

Some data are available on other lethal or sublethal effects on saltwater organisms (Table 3). The soft-shell clam, *Mya arenaria*, was exposed for 360 hr to nonylphenol concentrations up to 700 µg/L with no effects upon survival. Blue mussels, *Mytilus edulis*, were exposed for four days to two concentrations (100 and 1,130 µg/L) of nonylphenol and bioconcentrated the compound only 7.9 and 1.4 times, respectively, on a wet weight basis. Atlantic salmon similarily exposed for four days to 170 µg/L of nonylphenol bioconcentrated the compound 75 times on a wet weight basis. Experimentally derived bioconcentration values are not in agreement with calculated bioconcentration values (see Section III, General Information).

Calculation of Advisory Concentration

Due to the volatile nature of nonylphenol, data from static, unmeasured tests should not be used in the calculation of the advisory concentration. A total of four Species Mean Acute Values (SMAVs) and Genus Mean Acute Values (GMAVs) are available for freshwater and saltwater organisms combined (Table 3) from tests in which the concentrations of nonylphenol were measured. However, according to the guidelines (U.S. EPA 1987), another test is required to fulfill the requirement that another "species is either in the phylum Mollusca (and the test was begun as an embryo) or in a different family in the phylum Arthropoda."

A~~n~~ provisional advisory may be calculated with the available data as follows. The lowest GMAV (135 µg/L) is divided by a factor of 10.0, in accordance with the advisory guidelines, resulting in a provisional Advisory Acute Value (AAV) of 13.5 µg/L. The empirical acute-chronic ratio of 25 is used because there are no reported chronic tests. Division of the provisional AAV (13.5 µg/L) by the AACR (25) results in a provisional Advisory Concentration of 0.540 µg/L.

Table 1. Acute Toxicity of Nonylphenol to Aquatic Animals

FRESHWATER SPECIES

Species	Method[a]	Chemical[b]	Hardness (mg/L as $CaCO_3$)	LC50 or EC50 (µg/L)	Species Mean Acute Value (µg/L)	Reference
Fathead minnow (juvenile), *Pimephales promelas*	F, M	99%	45.1	LC50	135	Holcombe et al. 1984; Geiger et al. 1985

SALTWATER SPECIES

Species	Method[a]	Chemical[b]	Salinity (g/kg)	LC50 or EC50 (µg/L)	Species Mean Acute Value (µg/L)	Reference
Sand Shrimp, *Crangon septemspinosa*	R, M	Technical	-	LC50	300	McLeese et al. 1980b
Sand Shrimp, *Crangon septemspinosa*	R, M	-	-	LC50	300	McLeese et al. 1981
American lobster, *Homarus americanus*	R, M	-	-	LC50	170	McLeese et al. 1980b
Atlantic salmon (juvenile), *Salmo salar*	R, U	-	-	LC50	900	McLeese et al. 1980b

Table 1. (continued)

Species	Method[a]	Chemical	Salinity (g/kg)	LC50 or EC50 (ug/L)	Species Mean Acute Value (µg/L)	Reference
Atlantic salmon (juvenile), *Salmo salar*	R, M	-	-	LC50	190	McLeese et al. 1981
Atlantic salmon (juvenile), *Salmo salar*	F, M	-	-	LC50	160	McLeese et al. 1981
Atlantic salmon (juvenile), *Salmo salar*	F, M	Practical	-	LC50	130	McLeese et al. 1981

[a] S = Static; F = Flow-through; M = Measured; U = Unmeasured.

[b] Purity or grade of chemical is given when available.

Table 2. Ranked Genus Mean Acute Values with Species Mean Acute-Chronic Ratios

Rank[a]	Genus Mean Acute Value (µg/L)	Species	Species Mean Acute Value (µg/L)[b]	Species Mean Acute-Chronic Ratio[c]
4	300	Sand Shrimp, *Crangon septemspinosa*	300	-
3	170	American lobster, *Homarus americanus*	170	-
2	144.2	Atlantic salmon, *Salmo salar*	144.2	-
1	135	Fathead minnow, *Pimephales promelas*	135	-

[a] Ranked from most resistant to most sensitive based on Genus Mean Acute Value.

[b] From Table 1.

[c]

Advisory Acute Value = (135 µg/L) / 10.0 = 13.5 µg/L

Advisory Acute-Chronic Ratio = 25

Advisory Concentration = (13.5 µg/L) / 25 = 0.540 µg/L

Table 3. Other Data on Effects of Nonylphenol on Aquatic Organisms

FRESHWATER SPECIES

Species	Chemical[a]	Hardness (mg/L as $CaCO_3$)	Duration	Effect	Concentration (μg/L)	Reference
Clam, *Anadonta cataractae*	-	-	144 hr	LC50	1,700	McLeese et al. 1980b
Fathead minnow (juvenile), *Pimephales promelas*	99%	45.1	96 hr	Loss of equilibrium	98	Holcombe et al. 1984
Medaka, *Orizias latipes*	-	-	48 hr	LC50	4.36	Yoshioka et al. 1986

SALTWATER SPECIES

Species	Chemical[a]	Salinity (g/kg)	Duration	Effect	Concentration (μg/L)	Reference
Soft-shell clam, *Mya arenaria*	-	-	360 hr	LC50	> 700	McLeese et al. 1980b
Blue mussel, *Mytilus edulis*	-	-	4 day	BCF = 7.9	100	McLeese et al. 1980a
Blue mussel, *Mytilus edulis*	-	-	4 day	BCF = 1.4	1,130	McLeese et al. 1980a
Atlantic salmon, *Salmo salar*	Technical	-	4 day	BCF = 75	170	McLeese et al. 1981

[a] Percent purity or grade of chemical is listed when available.

REFERENCES

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