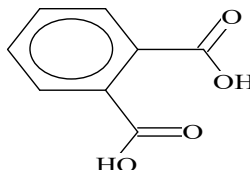


CAS Number: 000088-99-3  
SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
CHEM : O-PHTHALIC ACID  
MOL FOR: C8 H6 O4  
MOL WT : 166.13

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:

Log Kow (octanol-water): 0.73  
Boiling Point (deg C) : 324.85  
Melting Point (deg C) : 206.75  
Vapor Pressure (mm Hg) : 6.36E-007  
Water Solubility (mg/L): 6994  
Henry LC (atm-m3/mole) : -----



KOWWIN Program (v1.68) Results:

Log Kow(version 1.69 estimate): 1.07

Experimental Database Structure Match:

Name : O-PHTHALIC ACID  
CAS Num : 000088-99-3  
Exp Log P: 0.73  
Exp Ref : HANSCH,C ET AL. (1995)

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
CHEM : O-PHTHALIC ACID  
MOL FOR: C8 H6 O4  
MOL WT : 166.13

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	2	-COOH [acid, aromatic attach]	-0.1186	-0.2372
Factor	2	Ring reaction -> ortho to aromatic acid	-0.3425	-0.6850
Const		Equation Constant		0.2290
			Log Kow	= 1.0708

MPBPVP (v1.43) Program Results:

Experimental Database Structure Match:

Name : O-PHTHALIC ACID  
CAS Num : 000088-99-3  
Exp MP (deg C): 230 dec  
Exp BP (deg C): ---  
Exp VP (mm Hg): 6.36E-07 (extrapolated)  
(Pa ) : 8.48E-005  
Exp VP (deg C): 25  
Exp VP ref : DAUBERT,TE & DANNER,RP (1991)

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
CHEM : O-PHTHALIC ACID  
MOL FOR: C8 H6 O4  
MOL WT : 166.13

----- SUMMARY MPBPWIN v1.44 -----

Boiling Point: 351.37 deg C (Adapted Stein and Brown Method)

Melting Point: 266.90 deg C (Adapted Joback Method)

Melting Point: 91.50 deg C (Gold and Ogle Method)

Mean Melt Pt : 179.20 deg C (Joback; Gold,Ogle Methods)

Selected MP: 126.58 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):

(Using BP: 324.85 deg C (user entered))  
 (Using MP: 206.75 deg C (user entered))  
 VP: 3.82E-006 mm Hg (Antoine Method)  
   : 0.000509 Pa (Antoine Method)  
 VP: 6.13E-006 mm Hg (Modified Grain Method)  
   : 0.000817 Pa (Modified Grain Method)  
 VP: 1.59E-005 mm Hg (Mackay Method)  
   : 0.00212 Pa (Mackay Method)  
 Selected VP: 6.13E-006 mm Hg (Modified Grain Method)  
               : 0.000817 Pa (Modified Grain Method)  
 Subcooled liquid VP: 3.99E-005 mm Hg (25 deg C, user-entered VP )  
                       : 0.00532 Pa (25 deg C, user-entered VP )

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-COOH (acid)	169.83	339.66
Group	4	CH (aromatic)	28.53	114.12
Group	2	-C (aromatic)	30.76	61.52
*		Equation Constant		198.18
=====				
RESULT-uncorr		BOILING POINT in deg Kelvin		713.48
RESULT- corr		BOILING POINT in deg Kelvin		624.53
		BOILING POINT in deg C		351.37

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-COOH (acid)	155.50	311.00
Group	4	CH (aromatic)	8.13	32.52
Group	2	-C (aromatic)	37.02	74.04
*		Equation Constant		122.50
=====				
RESULT		MELTING POINT in deg Kelvin		540.06
		MELTING POINT in deg C		266.90

Water Sol from Kow (WSKOW v1.42) Results:

Water Sol: 8258 mg/L

Experimental Water Solubility Database Match:

Name : O-PHTHALIC ACID  
 CAS Num : 000088-99-3  
 Exp WSol : 6970 mg/L (25 deg C)  
 Exp Ref : YALKOWSKY,SH & HE,Y (2003)

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
 CHEM : O-PHTHALIC ACID  
 MOL FOR: C8 H6 O4  
 MOL WT : 166.13

----- WSKOW v1.43 Results -----  
 Log Kow (estimated) : 1.07  
 Log Kow (experimental): 0.73  
 Cas No: 000088-99-3  
 Name : O-PHTHALIC ACID  
 Refer : HANSCH,C ET AL. (1995)  
 Log Kow used by Water solubility estimates: 0.73 (user entered)

Equation Used to Make Water Sol estimate:

Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction

Melting Pt (Tm) = 206.75 deg C (Use Tm = 25 for all liquids)

Correction(s): Value

Acid, aromatic 0.898

Log Water Solubility (in moles/L) : -1.304

Water Solubility at 25 deg C (mg/L): 8258

WATERNT Program (v1.01) Results:

Water Sol (v1.01 est): 29678 mg/L

Experimental Water Solubility Database Match:

Name : O-PHTHALIC ACID  
CAS Num : 000088-99-3  
Exp WSol : 6970 mg/L (25 deg C)  
Exp Ref : YALKOWSKY, SH & HE, Y (2003)

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1

CHEM : O-PHTHALIC ACID

MOL FOR: C8 H6 O4

MOL WT : 166.13

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	Aromatic Carbon (C-H type)	-0.3359	-1.3435
Frag	2	-COOH [acid, aromatic attach]	0.0568	0.1136
Frag	2	Aromatic Carbon (C-substituent type)	-0.5400	-1.0799
Factor	2	Ring reaction -> ortho to aromatic acid	0.6563	1.3125
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -0.7480

Water Solubility (mg/L) at 25 dec C = 29678

ECOSAR Program (v1.11) Results:

ECOSAR Version 1.11 Results Page

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1

CHEM : O-PHTHALIC ACID

CAS Num:

ChemID1:

MOL FOR: C8 H6 O4

MOL WT : 166.13

Log Kow: 1.071 (EPISuite Kowwin v1.68 Estimate)

Log Kow: (User Entered)

Log Kow: 0.73 (PhysProp DB exp value - for comparison only)

Melt Pt: 206.75 (deg C, User Entered for Wat Sol estimate)

Melt Pt: 230.00 (deg C, PhysProp DB exp value for Wat Sol est, 230 dec)

Wat Sol: 8258 (mg/L, EPISuite WSKowwin v1.43 Estimate)

Wat Sol: 6994 (mg/L, User Entered)

Wat Sol: 6970 (mg/L, PhysProp DB exp value)

Values used to Generate ECOSAR Profile

Log Kow: 1.071 (EPISuite Kowwin v1.68 Estimate)

Wat Sol: 6994 (mg/L, User Entered)

ECOSAR v1.11 Class-specific Estimations

```

*****
| Not Related to an Existing ECOSAR Class Definition |
|
| Estimates provided below use the Neutral Organics QSAR equations which |
| represent baseline toxicity potential (minimum toxicity) assuming a simple |
| non-polar narcosis model. Without empirical data on structurally similar |
| chemicals, it is uncertain if this substance will present significantly |
| higher toxicity above baseline estimates. |
*****

```

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
--> Acid moiety found: Predicted values multiplied by 10				
Neutral Organics-acid	: Fish	96-hr	LC50	9323.396 *
Neutral Organics-acid	: Daphnid	48-hr	LC50	4858.623
Neutral Organics-acid	: Green Algae	96-hr	EC50	2538.352
Neutral Organics-acid	: Fish		ChV	823.613
Neutral Organics-acid	: Daphnid		ChV	373.177
Neutral Organics-acid	: Green Algae		ChV	549.129
Neutral Organics-acid	: Fish (SW)	96-hr	LC50	11672.349 *
Neutral Organics-acid	: Mysid	96-hr	LC50	16279.043 *
Neutral Organics-acid	: Fish (SW)		ChV	718.347
Neutral Organics-acid	: Mysid (SW)		ChV	1853.177
Neutral Organics-acid	: Earthworm	14-day	LC50	3605.933

Note: \* = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

#### Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

#### Neutral Organics:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)  
Maximum LogKow: 6.0 (Earthworm LC50)  
Maximum LogKow: 6.4 (Green Algae EC50)  
Maximum LogKow: 8.0 (ChV)

#### HENRYWIN (v3.20) Program Results:

Bond Est : 2.18E-012 atm-m3/mole (2.21E-007 Pa-m3/mole)  
Group Est: 3.88E-013 atm-m3/mole (3.93E-008 Pa-m3/mole)

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
CHEM : O-PHTHALIC ACID  
MOL FOR: C8 H6 O4  
MOL WT : 166.13

#### HENRYWIN v3.21 Results

#### Experimental Database Structure Match:

Name : O-PHTHALIC ACID  
CAS Num : 000088-99-3  
Exp HLC : 2.00E-11 atm-m3/mole (2.03E-006 Pa-m3/mole)

Temper : 25 deg C  
Exp Ref : VP/WSOL

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	4 Hydrogen to Carbon (aromatic) Bonds		-0.6172
HYDROGEN	2 Hydrogen to Oxygen Bonds		6.4635
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	2 Car-CO		2.4775
FRAGMENT	2 CO-O		0.1429
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	10.050

HENRYs LAW CONSTANT at 25 deg C = 2.18E-012 atm-m3/mole  
= 8.92E-011 unitless  
= 2.21E-007 Pa-m3/mole

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	4 Car-H (Car) (Car)		0.44
	2 Car (Car) (Car) (CO)		-1.68
	2 CO (O) (Car)		9.14
	2 O-H (CO)		2.90
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	10.80

HENRYs LAW CONSTANT at 25 deg C = 3.88E-013 atm-m3/mole  
= 1.58E-011 unitless  
= 3.93E-008 Pa-m3/mole

For Henry LC Comparison Purposes:

Exper Database: 2.00E-11 atm-m3/mole (2.03E-006 Pa-m3/mole)

User-Entered Henry LC: not entered

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 1.988E-011 atm-m3/mole (2.014E-006 Pa-m3/mole)

VP: 6.36E-007 mm Hg (source: User-Entered)

WS: 6.99E+003 mg/L (source: User-Entered)

Log Octanol-Air (KOAWIN v1.10) Results:

Log Koa: 9.817

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1

CHEM : O-PHTHALIC ACID

MOL FOR: C8 H6 O4

MOL WT : 166.13

----- KOAWIN v1.10 Results -----

Log Koa (octanol/air) estimate: 9.817

Koa (octanol/air) estimate: 6.568e+009

Using:

Log Kow: 0.73 (user entered)

HenryLC: 2e-011 atm-m3/mole (exp database)

Log Kaw: -9.087 (air/water part.coef.)

LogKow : 0.73 (exp database)

LogKow : 1.07 (KowWin estimate)

Henry LC: 2e-011 atm-m3/mole (exp database)

Henry LC: 2.18e-012 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 11.120 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
 CHEM : O-PHTHALIC ACID  
 MOL FOR: C8 H6 O4  
 MOL WT : 166.13

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Biodegrades Fast  
 Biowin2 (Non-Linear Model Prediction): Biodegrades Fast  
 Biowin3 (Ultimate Biodegradation Timeframe): Weeks  
 Biowin4 (Primary Biodegradation Timeframe): Days-Weeks  
 Biowin5 (MITI Linear Model Prediction) : Biodegrades Fast  
 Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast  
 Biowin7 (Anaerobic Model Prediction): Biodegrades Fast  
 Ready Biodegradability Prediction: YES

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic acid [-C(=O)-OH]	0.1769	0.3537
MolWt	*	Molecular Weight Parameter		-0.0791
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		1.0222

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic acid [-C(=O)-OH]	2.4224	4.8448
MolWt	*	Molecular Weight Parameter		-2.3591
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.9959

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic acid [-C(=O)-OH]	0.0879	0.1757
MolWt	*	Molecular Weight Parameter		-0.3671
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		3.0078

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic acid [-C(=O)-OH]	0.0077	0.0155
MolWt	*	Molecular Weight Parameter		-0.2397
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.6235

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks  
 (Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic acid [-C(=O)-OH]	0.3443	0.6886

Frag		4		Aromatic-H		0.0004		0.0016
MolWt		*		Molecular Weight Parameter				-0.2620
Const		*		Equation Constant				0.5544
=====								
RESULT				Biowin5 (MITI Linear Biodeg Probability)				0.9826
=====								

TYPE		NUM		Biowin6 FRAGMENT DESCRIPTION		COEFF		VALUE
-----								
Frag		2		Aromatic acid [-C(=O)-OH]		2.1403		4.2806
Frag		4		Aromatic-H		0.0342		0.1368
MolWt		*		Molecular Weight Parameter				-2.8741
=====								
RESULT				Biowin6 (MITI Non-Linear Biodeg Probability)				0.9610
=====								

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE		NUM		Biowin7 FRAGMENT DESCRIPTION		COEFF		VALUE
-----								
Frag		2		Aromatic acid [-C(=O)-OH]		0.2656		0.5311
Frag		4		Aromatic-H		-0.0954		-0.3817
Const		*		Equation Constant				0.8361
=====								
RESULT				Biowin7 (Anaerobic Linear Biodeg Prob)				0.9855
=====								

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is  $\geq 0.5$ , then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

BioHCwin (v1.01) Program Results:

=====

SMILES : O=C(O)c(c(cc1)C(=O)O)c1  
CHEM : O-PHTHALIC ACID  
MOL FOR: C8 H6 O4  
MOL WT : 166.13

----- BioHCwin v1.01 Results -----

NO Estimate Possible ... Structure NOT a Hydrocarbon  
(Contains atoms other than C, H or S (-S-))

AEROWIN Program (v1.00) Results:

=====

Sorption to aerosols (25 Dec C) [AEROWIN v1.00]:  
Vapor pressure (liquid/subcooled): 0.00532 Pa (3.99E-005 mm Hg)  
Log Koa (Koawin est ): 9.817  
Kp (particle/gas partition coef. (m3/ug)):

Mackay model : 0.000564  
Octanol/air (Koa) model: 0.00161  
Fraction sorbed to airborne particulates (phi):  
Junge-Pankow model : 0.02  
Mackay model : 0.0432  
Octanol/air (Koa) model: 0.114

AOP Program (v1.92) Results:

=====

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
CHEM : O-PHTHALIC ACID  
MOL FOR: C8 H6 O4  
MOL WT : 166.13

----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) -----

Hydrogen Abstraction	=	0.0000 E-12	cm3/molecule-sec
Reaction with N, S and -OH	=	1.0400 E-12	cm3/molecule-sec
Addition to Triple Bonds	=	0.0000 E-12	cm3/molecule-sec
Addition to Olefinic Bonds	=	0.0000 E-12	cm3/molecule-sec
Addition to Aromatic Rings	=	0.1970 E-12	cm3/molecule-sec
Addition to Fused Rings	=	0.0000 E-12	cm3/molecule-sec

OVERALL OH Rate Constant = 1.2370 E-12 cm3/molecule-sec  
HALF-LIFE = 8.647 Days (12-hr day; 1.5E6 OH/cm3)  
HALF-LIFE = 103.764 Hrs

----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----

\*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches  
Fraction sorbed to airborne particulates (phi):  
0.0316 (Junge-Pankow, Mackay avg)  
0.114 (Koa method)  
Note: the sorbed fraction may be resistant to atmospheric oxidation

KOCWIN Program (v2.00) Results:

=====

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
CHEM : O-PHTHALIC ACID  
MOL FOR: C8 H6 O4

Koc may be sensitive to pH!

-----

Experimental Database Structure Match:

Name : Phthalic acid  
CAS Num : 000088-99-3  
Exp LogKoc: 1.07  
Exp Ref : SRC (1991); Meylan et al (1992)

----- KOCWIN v2.01 Results -----

Koc Estimate from MCI:

-----

First Order Molecular Connectivity Index	.....	:	5.626
Non-Corrected Log Koc (0.5213 MCI + 0.60)	.....	:	3.5326
Fragment Correction(s):			
* Organic Acid (-CO-OH)	.....	:	-1.6249
Corrected Log Koc	.....	:	1.9077

Estimated Koc: 80.85 L/kg <=====

Koc Estimate from Log Kow:

-----

Log Kow (User entered)	.....	:	0.73
------------------------	-------	---	------

Non-Corrected Log Koc (0.55313 logKow + 0.9251) .... : 1.3289  
 Fragment Correction(s):  
     \* Organic Acid (-CO-OH) ..... : -0.7694  
 Corrected Log Koc ..... : 0.5595

Estimated Koc: 3.627 L/kg <=====

\*\*\*\*\*  
 \* NOTE: \*  
 \* The Koc of this structure may be sensitive to pH! The estimated \*  
 \* Koc represents a best-fit to the majority of experimental values \*  
 \* however, the Koc may vary significantly with pH. \*  
 \*\*\*\*\*

#### HYDROWIN Program (v2.00) Results:

=====

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
 CHEM : O-PHTHALIC ACID  
 MOL FOR: C8 H6 O4  
 MOL WT : 166.13

----- HYDROWIN v2.00 Results -----

Currently, this program can NOT estimate a hydrolysis rate constant for  
 the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),  
 Specific Alkyl Halides & Phosphorus Esters can be estimated!!

When present, various hydrolyzable compound-types will be identified.  
 For more information, (Click OVERVIEW in Help or see the User's Guide)

\*\*\*\*\* CALCULATION NOT PERFORMED \*\*\*\*\*

#### BCFBAF Program (v3.01) Results:

=====

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1  
 CHEM : O-PHTHALIC ACID  
 MOL FOR: C8 H6 O4  
 MOL WT : 166.13

----- BCFBAF v3.01 -----

#### Summary Results:

Log BCF (regression-based estimate): 0.50 (BCF = 3.16 L/kg wet-wt)  
 Biotransformation Half-Life (days) : 0.0793 (normalized to 10 g fish)  
 Log BAF (Arnot-Gobas upper trophic): 0.12 (BAF = 1.32 L/kg wet-wt)

Log Kow (experimental): 0.73  
 Log Kow used by BCF estimates: 0.73 (user entered)

Equation Used to Make BCF estimate:  
 Log BCF = 0.50 (Ionic; Log Kow dependent)

Estimated Log BCF = 0.500 (BCF = 3.162 L/kg wet-wt)

#### Whole Body Primary Biotransformation Rate Estimate for Fish:

TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic acid [-C(=O)-OH]	0.0000	0.0000
Frag	4	Aromatic-H	0.2664	1.0655

Frag		1		Benzene		-0.4277		-0.4277
L Kow		*		Log Kow = 0.73 (user-entered )		0.3073		0.2244
MolWt		*		Molecular Weight Parameter				-0.4260
Const		*		Equation Constant				-1.5371

---

RESULT				LOG Bio Half-Life (days)				-1.1009
RESULT				Bio Half-Life (days)				0.07926
NOTE				Bio Half-Life Normalized to 10 g fish at 15 deg C				

---

#### Biotransformation Rate Constant:

kM (Rate Constant): 8.745 /day (10 gram fish)  
 kM (Rate Constant): 4.918 /day (100 gram fish)  
 kM (Rate Constant): 2.765 /day (1 kg fish)  
 kM (Rate Constant): 1.555 /day (10 kg fish)

#### Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):

Estimated Log BCF (upper trophic) = 0.122 (BCF = 1.324 L/kg wet-wt)  
 Estimated Log BAF (upper trophic) = 0.122 (BAF = 1.324 L/kg wet-wt)  
 Estimated Log BCF (mid trophic) = 0.097 (BCF = 1.25 L/kg wet-wt)  
 Estimated Log BAF (mid trophic) = 0.097 (BAF = 1.25 L/kg wet-wt)  
 Estimated Log BCF (lower trophic) = 0.089 (BCF = 1.226 L/kg wet-wt)  
 Estimated Log BAF (lower trophic) = 0.089 (BAF = 1.226 L/kg wet-wt)

#### Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):

Estimated Log BCF (upper trophic) = 0.167 (BCF = 1.467 L/kg wet-wt)  
 Estimated Log BAF (upper trophic) = 0.169 (BAF = 1.475 L/kg wet-wt)

#### Volatilization From Water

---

Chemical Name: O-PHTHALIC ACID

Molecular Weight : 166.13 g/mole  
 Water Solubility : 6994 ppm  
 Vapor Pressure : 6.36E-007 mm Hg  
 Henry's Law Constant: 2E-011 atm-m3/mole (Henry experimental database)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	3.773E+007	4.116E+008
HALF-LIFE (days) :	1.572E+006	1.715E+007
HALF-LIFE (years) :	4304	4.696E+004

#### STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

---

(using 10000 hr Bio P,A,S)

#### PROPERTIES OF: O-PHTHALIC ACID

---

Molecular weight (g/mol)	166.13
Aqueous solubility (mg/l)	6994
Vapour pressure (Pa)	8.4793E-005
(atm)	8.36842E-010
(mm Hg)	6.36E-007
Henry 's law constant (Atm-m3/mol)	2E-011
Air-water partition coefficient	8.17941E-010
Octanol-water partition coefficient (Kow)	5.37032
Log Kow	0.73
Biomass to water partition coefficient	1.87406

Temperature [deg C] 25  
 Biodeg rate constants (h<sup>-1</sup>), half life in biomass (h) and in 2000 mg/L MLSS (h):  
 -Primary tank 0.02 37.34 10000.00  
 -Aeration tank 0.02 37.34 10000.00  
 -Settling tank 0.02 37.34 10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	6.0E-002	100.00
Primary sludge	2.62E-002	1.6E-004	0.26
Waste sludge	1.51E-001	9.1E-004	1.51
Primary volatilization	1.09E-008	6.6E-011	0.00
Settling volatilization	2.97E-008	1.8E-010	0.00
Aeration off gas	7.32E-008	4.4E-010	0.00
Primary biodegradation	1.76E-003	1.1E-005	0.02
Settling biodegradation	5.28E-004	3.2E-006	0.01
Aeration biodegradation	6.95E-003	4.2E-005	0.07
Final water effluent	9.81E+000	5.9E-002	98.13
Total removal	1.87E-001	1.1E-003	1.87
Total biodegradation	9.24E-003	5.6E-005	0.09

Level III Fugacity Model (Full-Output): User Koc

Chem Name : O-PHTHALIC ACID  
 Molecular Wt: 166.13  
 Henry's LC : 2e-011 atm-m3/mole (Henry database)  
 Vapor Press : 6.36e-007 mm Hg (user-entered)  
 Liquid VP : 3.99e-005 mm Hg (super-cooled)  
 Melting Pt : 207 deg C (user-entered)  
 Log Kow : 0.73 (user-entered)  
 Soil Koc : 11.7 (user-entered)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00445	208	1000
Water	8.7	72	0
Soil	91.3	144	0
Sediment	0.0145	648	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.2e-014	0.0279	0.0837	0.00279	0.00837
Water	9.85e-018	157	16.4	15.7	1.64
Soil	1.98e-015	826	0	82.6	0
Sediment	6.42e-018	0.0292	0.000547	0.00292	5.47e-005

Persistence Time: 188 hr  
 Reaction Time: 191 hr  
 Advection Time: 1.14e+004 hr  
 Percent Reacted: 98.4  
 Percent Advected: 1.64

Water Compartment Percents:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00445	208	1000
Water	8.7	72	0
water	(8.7)		
biota	(2.34e-006)		
suspended sediment	(0.000153)		

Soil	91.3	144	0
Sediment	0.0145	648	0

Half-Lives (hr), (based upon user-entry):

Air:	208
Water:	72
Soil:	144
Sediment:	648

Advection Times (hr):

Air:	100
Water:	1000
Sediment:	5e+004

Level III Fugacity Model (Full-Output): EQC Default

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Chem Name      : O-PHTHALIC ACID
Molecular Wt: 166.13
Henry's LC    : 2e-011 atm-m3/mole (Henry database)
Vapor Press   : 6.36e-007 mm Hg (user-entered)
Liquid VP     : 3.99e-005 mm Hg (super-cooled)
Melting Pt    : 207 deg C (user-entered)
Log Kow       : 0.73 (user-entered)
Soil Koc      : 2.2 (EQC Model Default)
  
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	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00457	208	1000
Water	11.1	72	0
Soil	88.9	144	0
Sediment	0.016	648	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.2e-014	0.0279	0.0837	0.00279	0.00837
Water	1.22e-017	195	20.3	19.5	2.03
Soil	3.09e-015	784	0	78.4	0
Sediment	8.39e-018	0.0314	0.000587	0.00314	5.87e-005

Persistence Time: 183 hr  
 Reaction Time: 187 hr  
 Advection Time: 9e+003 hr  
 Percent Reacted: 98  
 Percent Advected: 2.04

Water Compartment Percents:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00457	208	1000
Water	11.1	72	0
water	(11.1)		
biota	(2.97e-006)		
suspended sediment	(3.65e-005)		
Soil	88.9	144	0
Sediment	0.016	648	0

Half-Lives (hr), (based upon user-entry):

Air:	208
Water:	72
Soil:	144
Sediment:	648

Advection Times (hr):

Air:	100
Water:	1000
Sediment:	5e+004

