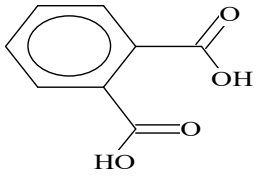
CAS Number: 000088-99-3
SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM : O-PHTHALIC ACID
MOL FOR: C8 H6 O4
MOL WT : 166.13

---------- 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.                               |
 ***************************************************************************

                                                                    Predicted
ECOSAR Class                  Organism            Duration  End Pt   mg/L (ppm)
============================  ==================  ========  ======   ==========
--> Acid moeity 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 >= 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(ccc1)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^-1),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	0.00174	208	1000
Water	24.6	72	1000
Soil	75.4	144	1000
Sediment	0.0411	648	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.2e-014	0.0279	0.0837	0.000929	0.00279
Water	7.11e-017	1.14e+003	118	37.9	3.94
Soil	4.17e-015	1.74e+003	0	58.1	0
Sediment	4.64e-017	0.211	0.00395	0.00704	0.000132

Persistence Time: 160 hr
Reaction Time: 167 hr
Advection Time: 4.06e+003 hr
Percent Reacted: 96.1
Percent Advected: 3.94

Water Compartment Percents:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00174	208	1000
Water	24.6	72	1000
water	(24.6)		
biota	(6.6e-006)		
suspended sediment	(0.000431)		

Soil	75.4	144	1000
Sediment	0.0411	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

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)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00178	208	1000
Water	26.9	72	1000
Soil	73.1	144	1000
Sediment	0.0389	648	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.2e-014	0.0279	0.0837	0.000929	0.00279
Water	7.61e-017	1.22e+003	126	40.6	4.22
Soil	6.52e-015	1.66e+003	0	55.2	0
Sediment	5.23e-017	0.196	0.00366	0.00653	0.000122

Persistence Time: 157 hr
Reaction Time: 164 hr
Advection Time: 3.72e+003 hr
Percent Reacted: 95.8
Percent Advected: 4.22

Water Compartment Percents:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00178	208	1000
Water	26.9	72	1000
water	(26.9)		
biota	(7.21e-006)		
suspended sediment	(8.87e-005)		
Soil	73.1	144	1000
Sediment	0.0389	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