The results output for Phthalic acid

a) Water Solubility

```
                Water Sol: 1.526e+004 mg/L
```

(Estimated value)

```
Experimental Water Solubility Database Match:
  Name     :  O-PHTHALIC ACID
  CAS Num  :  000088-99-3
  Exp WSol :  7010 mg/L (25 deg C)
  Exp Ref  :  YALKOWSKY,SH & DANNENFELSER,RM (1992)

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM   : 1,2-Benzenedicarboxylic acid
MOL FOR: C8 H6 O4
MOL WT : 166.13
----------------------------------WSKOW v1.41 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

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
      (used when Melting Point NOT available)

      Correction(s):         Value
      --------------------   -----
       Acid, aromatic        0.000

   Log Water Solubility  (in moles/L) :  -1.037
   Water Solubility at 25 deg C (mg/L):  1.526e+004

-------------------------------------------------------------------------
```

Program and version used

Equation used for the estimate

b) Partition coefficient n-octanol/water

```
                Log Kow(version 1.67 estimate): 1.07
```

(Estimated value)

```
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   : 1,2-Benzenedicarboxylic acid
MOL FOR: C8 H6 O4
MOL WT : 166.13

---------- KOWwin v1.67 Results ----------
```

Program and version used

```
-------+-----+-----------------------------------------+---------+--------
 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

--------------------------------------------------------------------------------
```

The method used to predict Kow. It is a fragment contribution method

C) Bioconcentration Factor (BCF)

Log BCF (v2.17 estimate): 0.50

```
SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM   : 1,2-Benzenedicarboxylic acid
MOL FOR: C8 H6 O4
MOL WT : 166.13
---------------------------------- Bcfwin v2.17 ---------------------
Log Kow  (estimated)  :  1.07
Log Kow (experimental):  0.73
Log Kow used by BCF estimates:  0.73

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


   Estimated Log BCF =  0.500  (BCF = 3.162)


--------------------------------------------------------------------------------
```

d) Soil Adsorption Coefficient (Koc/Kd)

Koc (estimated): 73.1

```
                Koc may be sensitive to pH!
SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM   : 1,2-Benzenedicarboxylic acid
MOL FOR: C8 H6 O4
MOL WT : 166.13
-------------------------- PCKOCWIN v1.66 Results -------------------------
--

         First Order Molecular Connectivity Index  ..... :  5.626
         Non-Corrected Log Koc  ........................... :  3.6149
         Fragment Correction(s):
                  *   Organic Acid  (-CO-OH)  ..............  : -1.7512
         Corrected Log Koc  ............................... :  1.8637

                        Estimated Koc:  73.06

                                  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.


--------------------------------------------------------------------------------
--
```

e) Henry's Law Constant

Two methods used to predict Henry's Constant

```
      Bond Est :  2.18E-012 atm-m3/mole
      Group Est:  3.88E-013 atm-m3/mole

SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM   : 1,2-Benzenedicarboxylic acid
MOL FOR: C8 H6 O4
MOL WT : 166.13
--------------------------- HENRYWIN v3.10 Results --------------------------
----------+-----------------------------------------------+---------+---------
   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

--------+-----------------------------------------------+------------+------
        |        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

------------------------------------------------------------------------------
```

(1)

(2)

f) Half lives-t1/2 for Hydrolysis as a function of Ph

Can not be estimated

g) Half lives-t1/2 for Photolysis (Atmospheric OH Rate Constant)

```
SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM   : 1,2-Benzenedicarboxylic acid
MOL FOR: C8 H6 O4
MOL WT : 166.13
------------------ SUMMARY (AOP v1.92): HYDROXYL RADICALS -----------------
--
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 -------------------

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

Experimental Database:  NO Structure Matches

---------------------------------------------------------------------------
```

h) Biodegradability

```
SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM   : 1,2-Benzenedicarboxylic 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)    :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Biodegrades Fast
   Ready Biodegradability Prediction:  YES
```

BIOWIN contains seven separate models to predict the biodegradation.

A brief summary of each model's prediction for Phthalic acid

This prediction is based on BIOWIN3 and 5 results.

Fragments used in each model to derive the estimation

```
------+-----+----------------------
 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
```

BIOWIN1 and 2 Results interpretation. For example, 0.99>0.5 so phthalic acid biodegrades 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
```

BIOWIN3 and 4 Results interpretation.

```
============+=============================================+=========+========
------+-----+---------------------------------------------+---------+--------
 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]                |  0.3770 |  0.7539
 Frag |  4  |  Aromatic-H                                 |  0.0082 |  0.0329
 MolWt|  *  |  Molecular Weight Parameter                 |         | -0.4942
 Const|  *  |  Equation Constant                          |         |  0.7121
============+=============================================+=========+========

   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)   |         |  1.0047
============+=============================================+=========+========

------+-----+---------------------------------------------+---------+--------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+--------
 Frag |  2  |  Aromatic acid   [-C(=O)-OH]                |  2.4449 |  4.8898
 Frag |  4  |  Aromatic-H                                 |  0.1201 |  0.4806
 MolWt|  *  |  Molecular Weight Parameter                 |         | -4.7961
============+=============================================+=========+========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.9569
============+=============================================+=========+========

 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
```

Fragments used in each model to derive the estimation

i) Aquatic toxicity

```
SMILES : O=C(O)c(c(ccc1)C(=O)O)c1
CHEM   : 1,2-Benzenedicarboxylic acid
CAS Num: 000088-99-3
ChemID1:
ChemID2:
ChemID3:
```

MOL FOR: C8 H6 O4
MOL WT : 166.13
Log Kow: 1.07 (KowWin estimate)
Melt Pt:
Wat Sol: 6562 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Neutral Organics-acid

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	1440.421
--> Acid moeity found: Predicted values multiplied by 10				
Neutral Organics-acid	: Fish	96-hr	LC50	9218.484 *
Neutral Organics-acid	: Fish	14-day	LC50	14404.213 *
Neutral Organics-acid	: Daphnid	48-hr	LC50	9263.168 *
Neutral Organics-acid	: Green Algae	96-hr	EC50	5489.205
Neutral Organics-acid	: Fish	30-day	ChV	1022.256
Neutral Organics-acid	: Daphnid	16-day	EC50	316.271
Neutral Organics-acid	: Green Algae	96-hr	ChV	320.686
Neutral Organics-acid	: Fish (SW)	96-hr	LC50	1346.975
Neutral Organics-acid	: Mysid Shrimp	96-hr	LC50	5163.683
				mg/kg (ppm) dry wt soil
Neutral Organics-acid	: Earthworm	14-day	LC50	19765.123 *

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

This defines the model domain for using ECOSAR to predict the aquatic toxicity of neutral organics acid. Basically, ECOSAR can be used to predict LC50(fish, Daphnid) for neutral organics with log Kow value<5.0 and MW<1000.