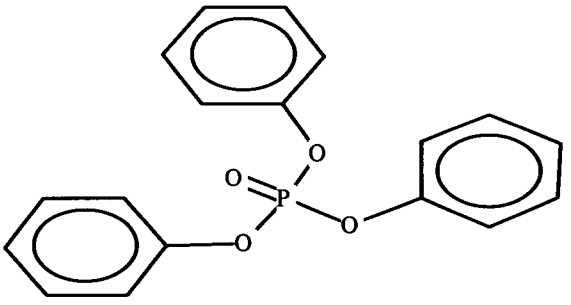

SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM : Phosphoric acid, triphenyl ester
CAS NUM: 000115-86-6
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29

---------- EPI SUMMARY (v3.12) ----------

Physical Property Inputs:

Water Solubility (mg/L):	------
Vapor Pressure (mm Hg) :	------
Henry LC (atm-m3/mole) :	------
Log Kow (octanol-water):	------
Boiling Point (deg C) :	------
Melting Point (deg C) :	------

KOWWIN Program (v1.67) Results:

Log Kow(version 1.67 estimate): 4.70

Experimental Database Structure Match:
Name : Triphenylphosphate
CAS Num : 000115-86-6
Exp Log P: 4.59
Exp Ref : Hansch,C et al. (1995)

SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	18	Aromatic Carbon	0.2940	5.2920
Frag	3	-O-P [aromatic attach]	0.5345	1.6035
Frag	1	O=P	-2.4239	-2.4239
Const		Equation Constant		0.2290
			Log Kow =	4.7006

MPBPWIN (v1.41) Program Results:

Experimental Database Structure Match:
Name : TRIPHENYLPHOSPHATE
CAS Num : 000115-86-6
Exp MP (deg C): 50.5
Exp BP (deg C): 245 @ 11 mm Hg
Exp VP (mm Hg): 6.28E-06 (extrapolated)
Exp VP (deg C): 25
Exp VP ref : DOBRY,A & KELLER,R (1957)

SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29

---------- SUMMARY MPBPWIN v1.41 ----------

Boiling Point: 441.27 deg C (Adapted Stein and Brown Method)

Melting Point: 75.00 deg C (Adapted Joback Method)
Melting Point: 143.99 deg C (Gold and Ogle Method)
Mean Melt Pt : 109.50 deg C (Joback; Gold,Ogle Methods)
Selected MP: 86.50 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 441.27 deg C (estimated))
(Using MP: 50.50 deg C (exp database))
VP: 4.07E-008 mm Hg (Antoine Method)
VP: 4.72E-007 mm Hg (Modified Grain Method)
VP: 9.5E-007 mm Hg (Mackay Method)
Selected VP: 4.72E-007 mm Hg (Modified Grain Method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	3	-O- (nonring)	25.16	75.48
Group	1	O=P<	107.23	107.23
Group	15	CH (aromatic)	28.53	427.95
Group	3	-C (aromatic)	30.76	92.28
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		901.12
RESULT- corr		BOILING POINT in deg Kelvin		714.43
		BOILING POINT in deg C		441.27

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	3	-O- (nonring)	22.23	66.69
Group	1	O=P<	50.00	50.00
Group	15	CH (aromatic)	8.13	121.95
Group	3	-C (aromatic)	37.02	111.06
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		472.20
Special-limit		MELTING POINT in deg Kelvin		348.16
		MELTING POINT in deg C		75.00

Water Sol from Kow (WSKOW v1.41) Results:

Water Sol: 1.034 mg/L

Experimental Water Solubility Database Match:
Name : TRIPHENYLPHOSPHATE
CAS Num : 000115-86-6
Exp WSol : 1.9 mg/L (25 deg C)
Exp Ref : SAEGER,VW ET AL. (1979)

SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29

---------- WSKOW v1.41 Results ----------

Log Kow (estimated) : 4.70
Log Kow (experimental): 4.59
Cas No: 000115-86-6
Name : Triphenylphosphate
Refer : Hansch,C et al. (1995)
Log Kow used by Water solubility estimates: 4.59

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

No Applicable Correction Factors

Log Water Solubility (in moles/L) : -5.499
Water Solubility at 25 deg C (mg/L): 1.034

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 4.6735 mg/L

Experimental Water Solubility Database Match:
Name : TRIPHENYLPHOSPHATE
CAS Num : 000115-86-6
Exp WSol : 1.9 mg/L (25 deg C)
Exp Ref : SAEGER,VW ET AL. (1979)

SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	15	Aromatic Carbon (C-H type)	-0.3359	-5.0380
Frag	3	Aromatic Carbon (C-substituent type)	-0.5400	-1.6199
Frag	3	-O-P [aromatic attach]	-0.5701	-1.7102
Frag	1	O=P	3.2748	3.2748
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -4.8440
Water Solubility (mg/L) at 25 dec C = 4.6735

ECOSAR Program (v0.99h) Results:
==========
SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM : Phosphoric acid, triphenyl ester
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29
Log Kow: 4.70 (KowWin estimate)
Melt Pt:
Wat Sol: 2.556 mg/L (calculated)

ECOSAR v0.99h Class(es) Found

Esters
Esters (phosphate)

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	Fish	14-day	LC50	1.949
Esters	Fish	96-hr	LC50	1.775
Esters	Daphnid	48-hr	LC50	0.905
Esters	Green Algae	96-hr	EC50	0.156
Esters	Green Algae		ChV	0.128
Esters	Fish		ChV	0.110
Esters (phosphate)	Fish	96-hr	LC50	1.024

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect.
Esters:
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
   Esters (phosphate):
      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



HENRY (v3.10) Program Results:
==============================

      Bond Est :  3.98E-008 atm-m3/mole
      Group Est:  Incomplete

SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM   : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29
--------------------------- HENRYWIN v3.10 Results --------------------------

Experimental Database Structure Match:
  Name     :  TRIPHENYLPHOSPHATE
  CAS Num  :  000115-86-6
  Exp HLC  :  3.31E-06 atm-m3/mole
  Temper   :  25 deg C
  Exp VP   :  6.28E-06 mm Hg
  Exp WSol :  1.90E+00 mg/L

----------+-----------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION       | COMMENT |  VALUE
----------+-----------------------------------------+---------+----------
 HYDROGEN |  15  Hydrogen to Carbon (aromatic) Bonds |         | -2.3144
 FRAGMENT |  18  Car-Car                            |         |  4.7485
 FRAGMENT |   3  O-P                                |         |  1.1791
 FRAGMENT |   1  O=P                                |         |  1.6334
 FRAGMENT |   3  Car-O                              |         |  1.0418
 FACTOR   |   1  Triaryl Phosphate group            |         | -0.5000
----------+-----------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE|  TOTAL  |  5.788
----------+-----------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 3.98E-008 atm-m3/mole
                               = 1.63E-006 unitless

--------+-----------------------------------------+-------------+--------
        |      GROUP CONTRIBUTION DESCRIPTION     |   COMMENT   |  VALUE
--------+-----------------------------------------+-------------+--------
        |          15  Car-H (Car)(Car)           |             |  1.65
        |           3  Car (Car)(Car)(O)          |             | -1.29
        |              MISSING Value for:  P (O)(O)(O)(=O)
        |              MISSING Value for:  O (Car)(P)
        |              MISSING Value for:  O (Car)(P)
        |              MISSING Value for:  O (Car)(P)
--------+-----------------------------------------+-------------+--------
 RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | INCOMPLETE |  0.36
--------+-----------------------------------------+-------------+--------

Henrys LC [VP/WSol estimate using EPI values]:
    HLC:  1.960E-007 atm-m3/mole
    VP:   4.72E-007 mm Hg
    WS:   1.03 mg/L



BIOWIN (v4.02) Program Results:
===============================
SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM   : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29
-------------------------- BIOWIN v4.02 Results -------------------------
```

Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction) : Does Not Biodegrade Fast
Biowin6 (MITI Non-Linear Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Phosphate ester	0.3139	0.3139
Frag	3	Unsubstituted phenyl group (C6H5-)	0.1281	0.3843
MolWt	*	Molecular Weight Parameter		-0.1553
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		1.2904

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Phosphate ester	44.4087	44.4087
Frag	3	Unsubstituted phenyl group (C6H5-)	1.7991	5.3973
MolWt	*	Molecular Weight Parameter		-4.6333
RESULT		Biowin2 (Non-Linear Biodeg Probability)		1.0000

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	1	Phosphate ester	0.1537	0.1537
Frag	3	Unsubstituted phenyl group (C6H5-)	0.0220	0.0660
MolWt	*	Molecular Weight Parameter		-0.7211
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.6979

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Phosphate ester	0.4654	0.4654
Frag	3	Unsubstituted phenyl group (C6H5-)	0.0049	0.0147
MolWt	*	Molecular Weight Parameter		-0.4708
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.8570

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	1	Phosphate ester	0.1547	0.1547
Frag	15	Aromatic-H	0.0082	0.1233
MolWt	*	Molecular Weight Parameter		-0.9707
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.0194

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Phosphate ester	1.1305	1.1305
Frag	15	Aromatic-H	0.1201	1.8021
MolWt	*	Molecular Weight Parameter		-9.4196

```
   RESULT    |Biowin6 (MITI Non-Linear Biodeg Probability)|          |  0.0187
=============+=============================================+=========+=========

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



AOP Program (v1.91) Results:
============================
SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM   : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29
------------------- SUMMARY (AOP v1.91): HYDROXYL RADICALS -------------------
Hydrogen Abstraction       =   0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 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 =  10.8423 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  10.8423 E-12 cm3/molecule-sec
   HALF-LIFE =     0.987 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =    11.838 Hrs
.......................  ** Designates Estimation(s) Using ASSUMED Value(s)
------------------- SUMMARY (AOP v1.91): OZONE REACTION ---------------------

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

Experimental Database:  NO Structure Matches



PCKOC Program (v1.66) Results:
==============================

                  Koc (estimated): 5.24e+003


SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM   : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29
------------------------------ PCKOCWIN v1.66 Results ------------------------------

         First Order Molecular Connectivity Index  ..... : 11.235
         Non-Corrected Log Koc  ........................... :  6.5972
         Fragment Correction(s):
                *   OrganoPhosphorus [P=O], aromatic ......  : -2.8781
         Corrected Log Koc  ............................... :  3.7191

                        Estimated Koc:  5237



HYDROWIN Program (v1.67) Results:
=================================
SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM   : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29
--------------------------- HYDROWIN v1.67 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)
   and Specific Alkyl Halides can be estimated!!  For more information,
    (Click OVERVIEW in Help  or  see the User's Guide)
```

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

BCF Program (v2.15) Results:
==========
SMILES : O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
CHEM : Phosphoric acid, triphenyl ester
MOL FOR: C18 H15 O4 P1
MOL WT : 326.29
---------- Bcfwin v2.15 ----------
Log Kow (estimated) : 4.70
Log Kow (experimental): 4.59
Log Kow used by BCF estimates: 4.59

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70 + Correction

Correction(s):	Value
Phosphate ester	-0.780

Estimated Log BCF = 2.054 (BCF = 113.3)

Volatilization From Water
==========

Chemical Name: Phosphoric acid, triphenyl ester

Molecular Weight : 326.29 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 3.31E-006 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) :	321.4	3657
HALF-LIFE (days) :	13.39	152.4

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
(using 10000 hr Bio P,A,S)
PROPERTIES OF: Phosphoric acid, triphenyl ester

Molecular weight (g/mol)	326.29
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry's law constant (Atm-m3/mol)	3.31E-006
Air-water partition coefficient	0.000135369
Octanol-water partition coefficient (Kow)	38904.5
Log Kow	4.59
Biomass to water partition coefficient	7781.71
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	9396.26	10000.00
-Aeration tank	0.00	9396.26	10000.00
-Settling tank	0.00	9396.26	10000.00

STP Overall Chemical Mass Balance:
---

	g/h	mol/h	percent
Influent	1.00E+001	3.1E-002	100.00
Primary sludge	3.66E+000	1.1E-002	36.58
Waste sludge	2.35E+000	7.2E-003	23.51

Primary volatilization	6.96E-004	2.1E-006	0.01
Settling volatilization	1.74E-003	5.3E-006	0.02
Aeration off gas	4.34E-003	1.3E-005	0.04
Primary biodegradation	1.14E-002	3.5E-005	0.11
Settling biodegradation	3.12E-003	9.6E-006	0.03
Aeration biodegradation	4.11E-002	1.3E-004	0.41
Final water effluent	3.93E+000	1.2E-002	39.29
Total removal	6.07E+000	1.9E-002	60.71
Total biodegradation	5.56E-002	1.7E-004	0.56

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

(using Biowin/EPA draft method)

PROPERTIES OF: Phosphoric acid, triphenyl ester

Molecular weight (g/mol)	326.29
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	3.31E-006
Air-water partition coefficient	0.000135369
Octanol-water partition coefficient (Kow)	38904.5
Log Kow	4.59
Biomass to water partition coefficient	7781.71
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	281.89	300.00
-Aeration tank	0.02	28.19	30.00
-Settling tank	0.02	28.19	30.00

STP Overall Chemical Mass Balance:

---

	g/h	mol/h	percent
Influent	1.00E+001	3.1E-002	100.00
Primary sludge	3.53E+000	1.1E-002	35.28
Waste sludge	6.79E-001	2.1E-003	6.79
Primary volatilization	6.71E-004	2.1E-006	0.01
Settling volatilization	5.02E-004	1.5E-006	0.01
Aeration off gas	1.26E-003	3.9E-006	0.01
Primary biodegradation	3.65E-001	1.1E-003	3.65
Settling biodegradation	3.01E-001	9.2E-004	3.01
Aeration biodegradation	3.99E+000	1.2E-002	39.89
Final water effluent	1.14E+000	3.5E-003	11.35
Total removal	8.86E+000	2.7E-002	88.65
Total biodegradation	4.66E+000	1.4E-002	46.55

Level III Fugacity Model (Full-Output):
==========

Chem Name : Phosphoric acid, triphenyl ester
Molecular Wt: 326.29
Henry's LC : 3.31e-006 atm-m3/mole (Henry database)
Vapor Press : 4.72e-007 mm Hg (Mpbpwin program)
Liquid VP : 1.92e-006 mm Hg (super-cooled)
Melting Pt : 86.5 deg C (Mpbpwin program)
Log Kow : 4.59 (Kowwin program)
Soil Koc : 1.6e+004 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.495	23.7	1000
Water	13.1	900	1000
Soil	74.3	1.8e+003	1000
Sediment	12.1	8.1e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.04e-011	599	205	20	6.82
Water	2.68e-011	417	542	13.9	18.1
Soil	4.52e-012	1.18e+003	0	39.5	0
Sediment	3.3e-011	42.7	9.98	1.42	0.333

Persistence Time: 1.38e+003 hr
Reaction Time: 1.84e+003 hr
Advection Time: 5.47e+003 hr
Percent Reacted: 74.8
Percent Advected: 25.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 23.68
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.698 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004