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QSAR Prediction Reporting Format (QPRF) for the estimation of the atmospheric hydroxyl radical rate constant and the hydroxyl radical reaction half-life for Triphenyl phosphate (CAS no. 115-86-6)

Summary

The rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and triphenyl phosphate and its atmospheric half-life was predicted using the Estimation Program Interface (EPI) Suite version 4.11.

The atmospheric rate constant was estimated to be 10.8423E-12 cm^3/molecule-sec. Considering an OH-concentration of 500000 radicals/cm^3 as a 24-h average, a half-life of 1.48 days was estimated.

1. SUBSTANCE:

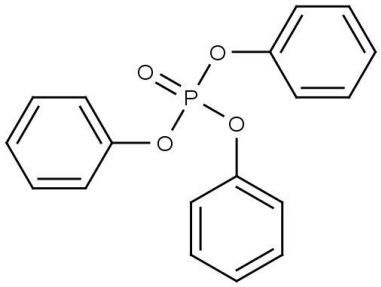
1.1 Chemical name: Triphenyl phosphate

1.2 CAS number: 115-86-6

1.3 EC number: 204-112-2

1.4 EC name: Triphenyl phosphate

1.5 Structural formula:



1.6 Empirical formula: $C_{18}H_{15}O_4P$

1.7 Structure codes:

- **a. SMILES:** O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
- **b. InChI:** 1S/C18H15O4P/c19-23(20-16-10-4-1-5-11-16,21-17-12-6-2-7-13-17)22-18-14-8-3-9-15-18/h1-15H
- **c. Other structural representation:** none
- **d. Stereo chemical features:** not applicable

1.8 Molecular weight: 326.29 g/mol

2. GENERAL INFORMATION

2.1 Date of QPRF: 2017-03-17

2.2 QPRF author and contact details: Dr. Susanne Dammers, Currenta GmbH & Co. OHG, Analytics, Product Safety / Ecotoxicology, CHEMPARK, Building Q18, 51368 Leverkusen (Germany)

3. PREDICTION

3.1 Endpoint (OECD Principle 1)

- **a. Endpoint:**

  Rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals at 25°C. The rate constant estimated by the program is then be used to calculate the atmospheric half-life for an organic compound based upon an 24h-day average atmospheric concentration of hydroxyl radicals of 5E+05 molecules/cm^3.

  Half-life is given in hours or days.

- **b. Dependent variable:**

  Hydroxyl radical rate constant in units of cm3/molecule-sec

3.2 Algorithm (OECD Principle 2)

a. Model or sub model name:

Individual model AOPWIN included in the Estimation Programs Interface (EPI) Suite.

b. Model version:

AOPWIN v1.92 included in EPI Suite v4.11, 2000 - 2012

c. Reference to QMRF

"QSAR Model Reporting Format (QMRF) for Indirect Photodegradation: Atmospheric Hydroxyl Radical Rate Constant and Hydroxyl Radical Reaction Half-Life", Currenta GmbH & Co. OHG, 01 September 2011

d. Predicted value (model result):

Atmospheric rate constant = 1.08423E-11 cm^3/molecule-sec

Half-life: 35.5 hours

e. Predicted value (comments):

The calculated value refers to the unaffected molecule. Any decomposition (e.g. hydrolysis) of the substance is not taken into account by the program.

f. Input for prediction:

A CAS number was entered in the initial data entry screen. In the structure window, the molecular weight, structural formula and the structure of the input SMILES notation is shown. If available, experimental determined values of melting point and boiling point are taken for input.

g. Descriptor values:

The molecule is separated into distinct fragments.

The reaction rate constant for hydroxyl radicals are the summation of the following mechanisms:

Hydrogen Abstraction	=	0 cm3/molecule*sec
Reaction with N, S and -OH	=	0 cm3/molecule*sec
Addition to Triple Bonds	=	0. cm3/molecule*sec
Addition to Olefinic Bonds	=	0 cm3/molecule*sec
**Addition to Aromatic Rings	=	1.08423E-11 cm3/molecule*sec
Addition to Fused Rings	=	0 cm3/molecule*sec

** Designates Estimation(s) Using ASSUMED Value(s)

As depending on the structure of the substance, OH-radicals generally react by one or more of the above mentioned pathways, the result of 0 cm3/molecule-sec for each mechanism indicate that these mechanisms are not relevant for the substance of interest.

An "assumed value" is applied, showing that a structure fragment that has not been assigned a numeric value by the developer of the estimation methods used by AOPWIN or derived explicitly from experimental values.

OH Addition to Aromatic Rings Calculation:

Most negative Es+ = -0.200

Log Kar = -11.71 - 1.34(Es+) cm3/molecule*sec

Ring #1 Kar = 3.6141E-12 cm3/molecule*sec

TOTAL Kar = 1.08423E-11 cm3/molecule*sec

Note: The bimolecular rate constant karom is expressed as Kar by the program.

3.3 Applicability domain (OECD principle 3)

a. Domains:

i. Molecular weight: not relevant

ii. Structural fragment domain:

Due to the fragment-based approach of AOPWIN, estimation is adequate as the fragments present in the molecule are available in the list of all fragment and reaction values provided by the program.

iii. Mechanism domain: no information available

iv. Metabolic domain, if relevant: not relevant

b. Structural analogues: no information available

c. Considerations on structural analogues: no information available

3.4 The uncertainty of the prediction (OECD principle 4)

Triphenyl phosphate is not highly complex and the applied rules appear appropriate. An individual uncertainty for the investigated substance is not available.

3.5 The chemical and biological mechanisms according to the model underpinning the predicted result (OECD principle 5).

No information available.

4. ADEQUACY (OPTIONAL)

4.1 Regulatory purpose:

The data may be used under any regulatory purpose.

4.2 Approach for regulatory interpretation of the model result:

If no experimental data are available the estimated value may be used to fill data gaps needed for hazard and risk assessment.

4.3 Outcome:

The prediction of the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and triphenyl phosphate and its atmospheric half-life yields useful results for further evaluation.

4.4 Conclusion:

The result is considered as useful for regulatory purposes.

Dr. Susanne Dammers

(Product Safety / Ecotoxicology)