

Phosphoric acid, tris(4-methylphenyl) ester

Other names:

Phosphoric acid, tri(4-tolyl) ester
Phosphoric acid, tri-p-tolyl ester
Tri-p-cresyl phosphate
Tri-p-tolyl phosphate
Tris(4-methylphenyl) phosphate
Tris(p-cresyl) phosphate
Tris(p-methylphenyl) phosphate
p-Tolyl phosphate ((C7H7O)3PO)
phosphoric acid, tri-p-cresyl ester
tri-4-tolyl phosphate

Inchi:

InChI=1S/C21H21O4P/c1-16-4-10-19(11-5-16)23-26(22,24-20-12-6-17(2)7-13-20)25-21-

InchiKey:

BOSMZFBHAYFUBJ-UHFFFAOYSA-N

Formula:

C21H21O4P

SMILES:

Cc1ccc(OP(=O)(Oc2ccc(C)cc2)Oc2ccc(C)cc2)cc1

Mol. weight [g/mol]:

368.36

CAS:

78-32-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.56		Crippen Method
logp	6.257		Crippen Method
mcvol	279.410	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	104.90	kJ/mol	459.00	NIST Webbook
pvap	1.10e-08	kPa	298.00	Determination of Vapor Pressures for Organophosphate Esters

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	4.01442e+01
Coeff. B	-3.31964e+04
Coeff. C	2.91764e+02
Temperature range (K), min.	541.12
Temperature range (K), max.	661.24

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of Vapor Pressures for Organophosphate Esters: McGowan Method:	https://www.doi.org/10.1021/je401026a
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure: Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78320&Units=SI https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure

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