Phosphoric acid, tris(2-methylphenyl) ester

Other names: NSC 438
Phosflex 179C
Phosphoric acid, tri-2-methylphenyl ester
Phosphoric acid, tri-o-cresyl ester
Phosphoric acid, tri-o-tolyl ester
TOCP
TOFK
TOTP
Tri-2-methylphenyl phosphate
Tri-2-tolyl phosphate
Tri-O-tolyl ester phosphoric acid
Tri-o-cresyl phosphate
Tri-o-tolyl phosphate
Tricresyl phosphate
Triorthocresyl phosphate
Tris(2-methylphenyl) phosphate
Tris(o-cresyl)-phosphate
Tris(o-methylphenyl)phosphate
Tris(o-tolyl) phosphate
Trojkrezylu fosforan
o-Cresyl phosphate
o-Tolyl phosphate
o-Trikresylphosphate
o-Trioyl phosphate

Inchi: InChI=1S/C21H21O4P/c1-16-10-4-7-13-19(16)23-26(22,24-20-14-8-5-11-17(20)2)25-21-

InchiKey: YSMRWXYRXBRSND-UHFFFAOYSA-N

Formula: C21H21O4P

SMILES: Cc1ccccc1OP(=O)(Oc1ccccc1C)Oc1ccccc1C

Mol. weight [g/mol]: 368.36

CAS: 78-30-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Aqueous Solubility Prediction Method
log10ws	-6.01		Estimated Solubility Method

logp	6.257		Crippen Method
mcvol	279.410	ml/mol	McGowan Method
ss	570.00	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	578.00	J/mol×K	298.15	NIST Webbook
hvapt	86.80	kJ/mol	496.50	NIST Webbook
pvap	5.10e-08	kPa	298.00	Determination of Vapor Pressures for Organophosphate Esters

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.08952e+01
Coeff. B	-8.70453e+03
Coeff. C	-1.07872e+02
Temperature range (K), min.	530.27
Temperature range (K), max.	666.44

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Determination of Vapor Pressures for Organophosphate Esters: https://www.doi.org/10.1021/je401026a

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78308&Units=SI

Legend

cps:	Solid phase heat capacity
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
ss:	Solid phase molar entropy at standard conditions