Phosphoric acid, tris(3-methylphenyl) ester

Other names:	NSC 4055
	Phosphoric acid, tri(3-tolyl) ester
	Phosphoric acid, tri-m-tolyl ester
	Tri-m-cresyl phosphate
	Tri-m-cresyl phosphite
	Tri-m-tolylphosphate
	Tris(m-tolyl) phosphate
	Tris-m-cresyl phosphate
	m-Tolyl phosphate, (C7H7O)3P
	tri-(3-methylphenyl) phosphate
	tri-m-tolyl phosphate
	tris-(3-methylphenyl) phosphate
Inchi:	InChI=1S/C21H21O4P/c1-16-7-4-10-19(13-16)23-26(22,24-20-11-5-8-17(2)14-20)25-21-
InchiKey:	RMLPZKRPSQVRAB-UHFFFAOYSA-N
Formula:	C21H21O4P
SMILES:	Cc1cccc(OP(=O)(Oc2cccc(C)c2)Oc2cccc(C)c2)c1
Mol. weight [g/mol]:	368.36
CAS:	563-04-2

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	123.20	kJ/mol	464.00	NIST Webbook
pvap	2.10e-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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C563042&Units=SI
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of Vapor Pressures for Organophosphate Esters:	https://www.doi.org/10.1021/je401026a

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