

Triisopropylphosphate

Other names:	Phosphoric acid, tris(1-methylethyl) ester Isopropyl phosphate, (C ₃ H ₇ O) ₃ PO Phosphoric acid, triisopropyl ester
Inchi:	InChI=1S/C ₉ H ₂₁ O ₄ P/c1-7(2)11-14(10,12-8(3)4)13-9(5)6/h7-9H,1-6H3
InchiKey:	OXFUXNFMHFCELM-UHFFFAOYSA-N
Formula:	C ₉ H ₂₁ O ₄ P
SMILES:	CC(C)OP(=O)(OC(C)C)OC(C)C
Mol. weight [g/mol]:	224.23
CAS:	513-02-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	3.370		Crippen Method
mcvol	181.610	ml/mol	McGowan Method
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1180.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C513020&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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