

Diisopropyl isobutyl phosphate

Inchi: InChI=1S/C10H23O4P/c1-8(2)7-12-15(11,13-9(3)4)14-10(5)6/h8-10H,7H2,1-6H3
InchiKey: JRBISAGZEVPIYCD-UHFFFAOYSA-N
Formula: C10H23O4P
SMILES: CC(C)COP(=O)(OC(C)C)OC(C)C
Mol. weight [g/mol]: 238.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.617		Crippen Method
mcvol	195.700	ml/mol	McGowan Method
rinpol	1317.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R403668&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/53-605-1/Diisopropyl-isobutyl-phosphate.pdf>

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