

Phosphoric acid, isoamyl-isooctyl ester

Inchi: InChI=1S/C13H29O4P/c1-12(2)8-6-5-7-10-16-18(14,15)17-11-9-13(3)4/h12-13H,5-11H2
InchiKey: RPXNGPMIXAZAKB-UHFFFAOYSA-N
Formula: C13H29O4P
SMILES: CC(C)CCCCCOP(=O)(O)OCCC(C)C
Mol. weight [g/mol]: 280.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	4.383		Crippen Method
mcvol	237.970	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=B6002065&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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