

Phenylphosphonic acid, isobutyl 2-methylpentyl ester

Inchi: InChI=1S/C16H27O3P/c1-5-9-15(4)13-19-20(17,18-12-14(2)3)16-10-7-6-8-11-16/h6-8,10
InchiKey: NJYLANRHNFIXJX-UHFFFAOYSA-N
Formula: C16H27O3P
SMILES: CCCC(C)COP(=O)(OCC(C)C)c1ccccc1
Mol. weight [g/mol]: 298.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.97		Crippen Method
logp	4.630		Crippen Method
mcvol	250.610	ml/mol	McGowan Method
rinpole	2100.00		NIST Webbook
rinpole	2100.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U393235&Units=SI>

Legend

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

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