

Phenylphosphonic acid, 2,4,4-trimethylpentyl propyl ester

Inchi: InChI=1S/C17H29O3P/c1-6-12-19-21(18,16-10-8-7-9-11-16)20-14-15(2)13-17(3,4)5/h7-17
InchiKey: RNTABEDZZHSJIZ-UHFFFAOYSA-N
Formula: C17H29O3P
SMILES: CCCOP(=O)(OCC(C)CC(C)(C)C)c1ccccc1
Mol. weight [g/mol]: 312.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.39		Crippen Method
logp	5.021		Crippen Method
mcvol	264.700	ml/mol	McGowan Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393218&Units=SI>
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>

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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