

Phenylphosphonic acid, 2-methylpentyl propyl ester

Inchi:	InChI=1S/C15H25O3P/c1-4-9-14(3)13-18-19(16,17-12-5-2)15-10-7-6-8-11-15/h6-8,10-11
InchiKey:	HQNCAROIKLCPKF-UHFFFAOYSA-N
Formula:	C15H25O3P
SMILES:	CCCOP(=O)(OCC(C)CCC)c1ccccc1
Mol. weight [g/mol]:	284.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.80		Crippen Method
logp	4.384		Crippen Method
mcvol	236.520	ml/mol	McGowan Method
rinpol	1920.00		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=U393248&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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