

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

Inchi:	InChI=1S/C16H27O3P/c1-6-18-20(17,15-10-8-7-9-11-15)19-13-14(2)12-16(3,4)5/h7-11,1
InchiKey:	FSTIMRJMCAA VFR-UHFFFAOYSA-N
Formula:	C16H27O3P
SMILES:	CCOP(=O)(OCC(C)CC(C)(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
rinpola	1933.00		NIST Webbook
rinpola	1933.00		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=U393232&Units=SI

Legend

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

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