

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

Inchi:	InChI=1S/C18H31O3P/c1-15(2)13-20-22(19,17-10-8-7-9-11-17)21-14-16(3)12-18(4,5)6/h
InchiKey:	ZEZVLPHQJRAYKO-UHFFFAOYSA-N
Formula:	C18H31O3P
SMILES:	CC(C)COP(=O)(OCC(C)CC(C)(C)C)c1ccccc1
Mol. weight [g/mol]:	326.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.57		Crippen Method
logp	5.266		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
rinpole	2049.00		NIST Webbook
rinpole	2049.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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