

Phenylphosphonic acid, hexyl 2-methylpentyl ester

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.05		Crippen Method
logp	5.555		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393264&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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