

Phenylphosphonic acid, isobutyl pentadecyl ester

Inchi:	InChI=1S/C25H45O3P/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-22-27-29(26,28-23-24(2)3)2
InchiKey:	IRBKDIRQAHDQSO-UHFFFAOYSA-N
Formula:	C25H45O3P
SMILES:	CCCCCCCCCCCCCOP(=O)(OCC(C)C)c1ccccc1
Mol. weight [g/mol]:	424.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.98		Crippen Method
logp	8.285		Crippen Method
mcvol	377.420	ml/mol	McGowan Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		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=U393267&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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