

Phenylphosphonic acid, isobutyl tridecyl ester

Inchi: InChI=1S/C23H41O3P/c1-4-5-6-7-8-9-10-11-12-13-17-20-25-27(24,26-21-22(2)3)23-18-
InchiKey: QRABQWVFPPJZFF-UHFFFAOYSA-N
Formula: C23H41O3P
SMILES: CCCCCCCCCCCCOP(=O)(OCC(C)C)c1ccccc1
Mol. weight [g/mol]: 396.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.15		Crippen Method
logp	7.505		Crippen Method
mcvol	349.240	ml/mol	McGowan Method
rinpol	2729.00		NIST Webbook
rinpol	2729.00		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=U393253&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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