

Phenylphosphonic acid, hexyl ethyl ester

Inchi: InChI=1S/C14H23O3P/c1-3-5-6-10-13-17-18(15,16-4-2)14-11-8-7-9-12-14/h7-9,11-12H,3
InchiKey: LXVXKGGJTEWMLSN-UHFFFAOYSA-N
Formula: C14H23O3P
SMILES: CCCCCCOP(=O)(OCC)c1ccccc1
Mol. weight [g/mol]: 270.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.62		Crippen Method
logp	4.138		Crippen Method
mcvol	222.430	ml/mol	McGowan Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393215&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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