

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

Inchi: InChI=1S/C28H51O3P/c1-6-7-8-9-10-11-12-13-14-15-16-20-23-30-32(29,27-21-18-17-19)
InchiKey: VFZGYNQLDKCMFR-UHFFFAOYSA-N
Formula: C28H51O3P
SMILES: CCCCCCCCCCCCCOP(=O)(OCC(C)CC(C)(C)C)c1ccccc1
Mol. weight [g/mol]: 466.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.00		Crippen Method
logp	9.312		Crippen Method
mcvol	419.690	ml/mol	McGowan Method
rinpol	3087.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393229&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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