

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

Inchi: InChI=1S/C22H39O3P/c1-6-7-8-9-10-14-17-24-26(23,21-15-12-11-13-16-21)25-19-20(2)
InchiKey: MUHLFZNMHULFIN-UHFFFAOYSA-N
Formula: C22H39O3P
SMILES: CCCCCCOP(=O)(OCC(C)CC(C)(C)C)c1cccc1
Mol. weight [g/mol]: 382.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.49		Crippen Method
logp	6.971		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
rinpole	2488.00		NIST Webbook
rinpole	2488.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393223&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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