

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

Inchi: InChI=1S/C21H37O3P/c1-6-7-8-9-13-16-23-25(22,20-14-11-10-12-15-20)24-18-19(2)17-
InchiKey: HALLRGAELMVYRC-UHFFFAOYSA-N
Formula: C21H37O3P
SMILES: CCCCCCOP(=O)(OCC(C)CC(C)(C)C)c1ccccc1
Mol. weight [g/mol]: 368.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.07		Crippen Method
logp	6.581		Crippen Method
mcvol	321.060	ml/mol	McGowan Method
rinpole	2390.00		NIST Webbook
rinpole	2390.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393222&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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