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

Inchi: InChI=1S/C19H33O3P/c1-6-7-11-14-21-23(20,18-12-9-8-10-13-18)22-16-17(2)15-19(3,4

InchiKey: MDXRZQIAEGNFCH-UHFFFAOYSA-N

Formula: C19H33O3P

SMILES: CCCCCOP(=O)(OCC(C)CC(C)(C)C)c1ccccc1

Mol. weight [g/mol]: 340.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.23		Crippen Method
logp	5.801		Crippen Method
mcvol	292.880	ml/mol	McGowan Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393221&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.