Phenylphosphonic acid, 2-methylpentyl pentyl ester

Inchi: InChI=1S/C17H29O3P/c1-4-6-10-14-19-21(18,17-12-8-7-9-13-17)20-15-16(3)11-5-2/h7-9

InchiKey: IWHXGYZDNYCRCI-UHFFFAOYSA-N

Formula: C17H29O3P

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

Mol. weight [g/mol]: 312.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.63		Crippen Method
logp	5.165		Crippen Method
mcvol	264.700	ml/mol	McGowan Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook

Sources

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

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=U393266&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

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