Phenylphosphonic acid, heptyl 2-methylpentyl ester

Inchi: InChI=1S/C19H33O3P/c1-4-6-7-8-12-16-21-23(20,19-14-10-9-11-15-19)22-17-18(3)13-5

InchiKey: NCGWXDUHIFHGPN-UHFFFAOYSA-N

Formula: C19H33O3P

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

Mol. weight [g/mol]: 340.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.47		Crippen Method
logp	5.945		Crippen Method
mcvol	292.880	ml/mol	McGowan Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393263&Units=SI

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

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.