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

Inchi: InChI=1S/C29H53O3P/c1-6-7-8-9-10-11-12-13-14-15-16-17-21-24-31-33(30,28-22-19-18
InchiKey: FJUNUOCVAFOESZ-UHFFFAOYSA-N
Formula: C29H53O3P
SMILES: CCCCCCCCCCCCCCCOP(=O)(OCC(C)CC(C)(C)C)c1ccccc1
Mol. weight [g/mol]: 480.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.42		Crippen Method
logp	9.702		Crippen Method
mcvol	433.780	ml/mol	McGowan Method
rinpol	3187.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393230&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