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

Inchi: InChI=1S/C26H47O3P/c1-6-7-8-9-10-11-12-13-14-18-21-28-30(27,25-19-16-15-17-20-25

InchiKey: LJZZLAIGEUPHHJ-UHFFFAOYSA-N

Formula: C26H47O3P

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

Mol. weight [g/mol]: 438.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.16		Crippen Method
logp	8.531		Crippen Method
mcvol	391.510	ml/mol	McGowan Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393227&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.