Phenylphosphonic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C22H39O3P/c1-18(14-21(3,4)5)16-24-26(23,20-12-10-9-11-13-20)25-17-19(2)15-22(6,7)8/h9-13,18-19H,14-17H2,1-8H3

InchiKey: DFBOPFGDUIJQCX-UHFFFAOYSA-N

Formula: C22H39O3P

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

Mol. weight [g/mol]: 382.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.00		Crippen Method
logp	6.683		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393231&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.