Phenylphosphonic acid, pentadecyl pentyl ester

Inchi: InChI=1S/C26H47O3P/c1-3-5-7-8-9-10-11-12-13-14-15-16-21-25-29-30(27,28-24-20-6-4

InchiKey: GZRMLCRRDCHDNC-UHFFFAOYSA-N

Formula: C26H47O3P

SMILES: CCCCCCCCCCCCCCCCOP(=O)(OCCCCC)c1ccccc1

Mol. weight [g/mol]: 438.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.64		Crippen Method
logp	8.820		Crippen Method
mcvol	391.510	ml/mol	McGowan Method
rinpol	3073.00		NIST Webbook
rinpol	3073.00		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=U393269&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.