Phenylphosphonic acid, hexyl tridecyl ester

Inchi: InChI=1S/C25H45O3P/c1-3-5-7-9-10-11-12-13-14-15-20-24-28-29(26,25-21-17-16-18-22
InchiKey: RMHABUYIGYOXNF-UHFFFAOYSA-N
Formula: C25H45O3P
SMILES: CCCCCCCCCCCCCOP(=O)(OCCCCCC)c1ccccc1
Mol. weight [g/mol]: 424.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-14.23		Crippen Method
logp	8.429		Crippen Method
mcvol	377.420	ml/mol	McGowan Method
rinpol	2966.00		NIST Webbook
rinpol	2966.00		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=U393256&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.