Phenylphosphonic acid, di(4-octyl) ester

Inchi: InChI=1S/C22H39O3P/c1-5-9-16-20(14-7-3)24-26(23,22-18-12-11-13-19-22)25-21(15-8-
InchiKey: QLRPJUNZXPDZCW-UHFFFAOYSA-N
Formula: C22H39O3P
SMILES: CCCCC(CCC)OP(=O)(OC(CCC)CCCC)c1ccccc1
Mol. weight [g/mol]: 382.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.19		Crippen Method
logp	7.256		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		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=U393238&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.