Phenylphosphonic acid, dodecyl propyl ester

Inchi: InChI=1S/C21H37O3P/c1-3-5-6-7-8-9-10-11-12-16-20-24-25(22,23-19-4-2)21-17-14-13-1
InchiKey: OBHGNTMZSMACDP-UHFFFAOYSA-N
Formula: C21H37O3P
SMILES: CCCCCCCCCCCCOP(=O)(OCCC)c1ccccc1
Mol. weight [g/mol]: 368.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.55		Crippen Method
logp	6.869		Crippen Method
mcvol	321.060	ml/mol	McGowan Method
rinpol	2610.00		NIST Webbook
rinpol	2610.00		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=U393240&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.