Phenylphosphonic acid, pentyl tridecyl ester

Inchi: InChI=1S/C24H43O3P/c1-3-5-7-8-9-10-11-12-13-14-19-23-27-28(25,26-22-18-6-4-2)24-2
InchiKey: NZYUWZRXFSRTDJ-UHFFFAOYSA-N
Formula: C24H43O3P
SMILES: CCCCCCCCCCCCCOP(=O)(OCCCCC)c1ccccc1
Mol. weight [g/mol]: 410.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.81		Crippen Method
logp	8.039		Crippen Method
mcvol	363.330	ml/mol	McGowan Method
rinpol	2874.00		NIST Webbook
rinpol	2874.00		NIST Webbook

Sources

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=U393255&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.