

Phenylphosphonic acid, ethyl hexadecyl ester

Inchi: InChI=1S/C24H43O3P/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-20-23-27-28(25,26-4-2)24-2
InchiKey: PTUMKMLVEDNJCU-UHFFFAOYSA-N
Formula: C24H43O3P
SMILES: CCCCCCCCCCCCCCOP(=O)(OCC)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
rinpole	2928.00		NIST Webbook
rinpole	2928.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393260&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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