

Phenylphosphonic acid, dodecyl heptyl ester

Inchi: InChI=1S/C25H45O3P/c1-3-5-7-9-10-11-12-13-15-20-24-28-29(26,25-21-17-16-18-22-25)
InchiKey: LREJQGUIXXJNOI-UHFFFAOYSA-N
Formula: C25H45O3P
SMILES: CCCCCCCCCCOP(=O)(OCCCCCCC)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
rinpole	2968.00		NIST Webbook
rinpole	2968.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U393245&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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