

Phenylphosphonic acid, 4-octyl propyl ester

Inchi: InChI=1S/C17H29O3P/c1-4-7-12-16(11-5-2)20-21(18,19-15-6-3)17-13-9-8-10-14-17/h8-17
InchiKey: PHGLLPGYZMLYSK-UHFFFAOYSA-N
Formula: C17H29O3P
SMILES: CCCCC(CCC)OP(=O)(OCCC)c1ccccc1
Mol. weight [g/mol]: 312.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.99		Crippen Method
logp	5.307		Crippen Method
mcvol	264.700	ml/mol	McGowan Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		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=U393233&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

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