

Butamifos oxon

Inchi: InChI=1S/C13H21N2O5P/c1-5-11(4)14-21(18,19-6-2)20-13-9-10(3)7-8-12(13)15(16)17/h
InchiKey: KTBHXCBJYRPDHP-UHFFFAOYSA-N
Formula: C13H21N2O5P
SMILES: CCOP(=O)(NC(C)CC)Oc1cc(C)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 316.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	3.815		Crippen Method
mcvol	235.740	ml/mol	McGowan Method
rinpol	2086.00		NIST Webbook
rinpol	2086.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R197378&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

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<https://www.chemeo.com/cid/112-636-1/Butamifos-oxon.pdf>

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