

EPN OXON

Inchi: InChI=1S/C14H14NO5P/c1-2-19-21(18,14-6-4-3-5-7-14)20-13-10-8-12(9-11-13)15(16)17
InchiKey: PDABPGQGULTJFY-UHFFFAOYSA-N
Formula: C14H14NO5P
SMILES: CCOP(=O)(Oc1ccc([N+](=O)[O-])cc1)c1ccccc1
Mol. weight [g/mol]: 307.24
CAS: 2012-00-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.02		Crippen Method
logp	3.529		Crippen Method
mcvol	216.090	ml/mol	McGowan Method
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C2012002&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

Latest version available from:

<https://www.chemeo.com/cid/89-909-5/EPN-OXON.pdf>

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