

Amisometradine

Inchi: InChI=1S/C9H13N3O2/c1-6(2)5-12-7(10)4-8(13)11(3)9(12)14/h4H,1,5,10H2,2-3H3
InchiKey: FXNYSZHYMGWWEZ-UHFFFAOYSA-N
Formula: C9H13N3O2
SMILES: C=C(C)Cn1c(N)cc(=O)n(C)c1=O
Mol. weight [g/mol]: 195.22
CAS: 550-28-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	-0.295		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
rinpol	2021.00		NIST Webbook
rinpol	2021.00		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=C550287&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/20-824-4/Amisometradine.pdf>

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