

AJMALINE, AC

Inchi: InChI=1S/C24H30N2O4/c1-5-14-15-10-18-21-24(16-8-6-7-9-17(16)25(21)4)11-19(20(15)
InchiKey: GSRQQKLTXCUIFV-UHFFFAOYSA-N
Formula: C24H30N2O4
SMILES: CCC1C2CC3C4N(C)c5ccccc5C45CC(C2C5OC(C)=O)N3C1OC(C)=O
Mol. weight [g/mol]: 410.51
CAS: 19775-56-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.696		Crippen Method
mcvol	305.800	ml/mol	McGowan Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		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=C19775565&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/95-600-0/AJMALINE-AC.pdf>

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