Ammodendrine

Inchi: InChI=1S/C12H20N2O/c1-10(15)14-8-4-5-11(9-14)12-6-2-3-7-13-12/h9,12-13H,2-8H2,1H
InchiKey: APKLQIQRPUDADG-UHFFFAOYSA-N
Formula: C12H20N2O
SMILES: CC(=O)N1C=C(C2CCCCN2)CCC1
Mol. weight [g/mol]: 208.30
CAS: 494-15-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Crippen Method
logp	1.655		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1863.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1865.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C494155&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices