Tashiromine

Inchi: InChI=1S/C9H17NO/c11-7-8-3-1-5-10-6-2-4-9(8)10/h8-9,11H,1-7H2/t8-,9-/m0/s1
InchiKey: DATGBSBEMJWBMW-IUCAKERBSA-N
Formula: C9H17NO
SMILES: OCC1CCCN2CCCC12
Mol. weight [g/mol]: 155.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	0.853		Crippen Method
mcvol	131.800	ml/mol	McGowan Method
rinpol	1280.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook

Sources

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=R261211&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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