AJMALINE, M(HO-), AC

Inchi: InChI=1S/C26H32N2O6/c1-6-16-17-10-20-23-26(18-9-15(32-12(2)29)7-8-19(18)27(23)5)
InchiKey: IQBHXEBPPOSIQT-AOSISCJSSA-N
Formula: C26H32N2O6
SMILES: CCC1C2CC3C4N(C)c5ccc(OC(C)=O)cc5C45CC(C2C5OC(C)=O)N3C1OC(C)=O
Mol. weight [g/mol]: 468.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.13		Crippen Method
logp	2.621		Crippen Method
mcvol	341.420	ml/mol	McGowan Method
rinpol	3100.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R254981&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