N-Acetylnorlaudanosine

Inchi: InChI=1S/C22H27NO5/c1-14(24)23-9-8-16-12-21(27-4)22(28-5)13-17(16)18(23)10-15-6-
InchiKey: JIDKUPJJVWNDTF-SFHVURJKSA-N
Formula: C22H27NO5
SMILES: COc1ccc(CC2c3cc(OC)c(OC)cc3CCN2C(C)=O)cc1OC
Mol. weight [g/mol]: 385.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	3.409		Crippen Method
mcvol	297.490	ml/mol	McGowan Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		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=R330837&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.