Laudanosine

Inchi: InChI=1S/C21H27NO4/c1-22-9-8-15-12-20(25-4)21(26-5)13-16(15)17(22)10-14-6-7-18(2
InchiKey: KGPAYJZAMGEDIQ-UHFFFAOYSA-N
Formula: C21H27NO4
SMILES: COc1ccc(CC2c3cc(OC)c(OC)cc3CCN2C)cc1OC
Mol. weight [g/mol]: 357.44
CAS: 20412-65-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	3.493		Crippen Method
mcvol	281.830	ml/mol	McGowan Method
rinpol	2660.00		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=C20412651&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.