Phyllalbine

Inchi: InChI=1S/C16H21NO4/c1-17-11-4-5-12(17)9-13(8-11)21-16(19)10-3-6-14(18)15(7-10)20
InchiKey: OZKTVDIYALBSMA-UHFFFAOYSA-N
Formula: C16H21NO4
SMILES: COc1cc(C(=O)OC2CC3CCC(C2)N3C)ccc1O
Mol. weight [g/mol]: 291.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	2.183		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R510197&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.