Feruloyliupinine

Inchi: InChI=1S/C20H27NO4/c1-24-19-13-15(7-9-18(19)22)8-10-20(23)25-14-16-5-4-12-21-11-
InchiKey: PWEDVDRRTZZEER-PFSJMHODSA-N
Formula: C20H27NO4
SMILES: COc1cc(C=CC(=O)OCC2CCCN3CCCCC23)ccc1O
Mol. weight [g/mol]: 345.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	3.222		Crippen Method
mcvol	272.040	ml/mol	McGowan Method
rinpol	2960.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R308499&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