p-Coumaroyllupinine

Inchi: InChI=1S/C19H25NO3/c21-17-9-6-15(7-10-17)8-11-19(22)23-14-16-4-3-13-20-12-2-1-5-
InchiKey: IZIOGYPZZKPZLM-KDVLCQBISA-N
Formula: C19H25NO3
SMILES: O=C(C=Cc1ccc(O)cc1)OCC1CCCN2CCCCC12
Mol. weight [g/mol]: 315.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	3.213		Crippen Method
mcvol	252.080	ml/mol	McGowan Method
rinpol	2860.00		NIST Webbook
rinpol	2860.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R308513&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

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