(S)-Laudanine

Inchi:	InChI=1S/C20H25NO4/c1-21-8-7-14-11-19(24-3)20(25-4)12-15(14)16(21)9-13-5-6-18(23
InchiKey:	MPYHGNAJOKCMAQ-MRXNPFEDSA-N
Formula:	C20H25NO4
SMILES:	COc1ccc(CC2c3cc(OC)c(OC)cc3CCN2C)cc1O
Mol. weight [g/mol]:	343.42
CAS:	3122-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	3.190		Crippen Method
mcvol	267.740	ml/mol	McGowan Method
rinpol	2784.80		NIST Webbook
rinpol	2784.80		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3122950&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

Latest version available from:
https://www.chemeo.com/cid/96-438-0/S-Laudanine.pdf