11-EPIHEMANTHAMINE

Other names:	11-Epihemanthamine
	12-Epihemanthamine
	3-Methoxy-1,2-didehydrocrinan-11-ol-, (3«beta»,5«alpha»,11S,13«beta»,19«alpha»)-
	haemanthamine
Inchi:	InChI=1S/C17H19NO4/c1-20-11-2-3-17-12-6-14-13(21-9-22-14)4-10(12)7-18(8-16(17)19
InchiKey:	YGPRSGKVLATIHT-UHFFFAOYSA-N
Formula:	C17H19NO4
SMILES:	COC1C=CC23c4cc5c(cc4CN(CC2O)C3C1)OCO5
Mol. weight [g/mol]:	301.34

Physical Properties

Property code	Value	Unit	Source
logp	1.187		Crippen Method
mcvol	212.350	ml/mol	McGowan Method
rinpol	2585.00		NIST Webbook

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1472760&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices