Crinan-11-ol, 1,2-didehydro-3-methoxy-, (3«beta»,5«alpha»,11R,13«beta»,19«alpha»)-

Other names: 4a«beta»,5«alpha»,11b«alpha»-Crinan-12-ol, 1,2-didehydro-3«beta»-methoxy-, (12R)-
Crinan-18-ol, 1,2-didehydro-3-methoxy-, (3«beta»,5«beta»,6«alpha»,17«alpha»,18R)-
Natalensin
Natalensine
3-Epicrinamine
3H,6H-5,11b-Ethano[1,3]dioxolo[4,5-j]phenanthridine, crinan-18-ol deriv.
(3S,4aS,5S,11bS,12R)-3-Methoxy-3,4,4a,6-tetrahydro-11b,5-ethano[1,3]dioxolo[4,5-j]phe

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

CAS: 466-75-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	1.187		Crippen Method
mcvol	212.350	ml/mol	McGowan Method
rinpol	2639.10		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C466751&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices