Galanthan-1-ol, 3,12-didehydro-2,9,10-trimethoxy-, (1«alpha»,2«beta»)-

Other names: Galanthine
9,10-Secolycoran-1«alpha»-ol, 3,3a-didehydro-2«beta»-methoxy-O9-methyl-
2,9,10-Trimethoxy-3,12-didehydrogalanthan-1-ol-, (1«alpha»,2«beta»)-
(1S,2S,3a1S,11bS)-2,9,10-Trimethoxy-2,3a1,4,5,7,11b-hexahydro-1H-pyrrolo[3,2,1-de]ph
Inchi: InChI=1S/C18H23NO4/c1-21-13-7-11-9-19-5-4-10-6-15(23-3)18(20)16(17(10)19)12(11)8
InchiKey: VOIMPDXOQJYVDI-UHFFFAOYSA-N
Formula: C18H23NO4
SMILES: COc1cc2c(cc1OC)C1C(O)C(OC)C=C3CCN(C2)C31
Mol. weight [g/mol]: 317.38
CAS: 517-78-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	1.691		Crippen Method
mcvol	237.300	ml/mol	McGowan Method
rinpol	2722.20		NIST Webbook
rinpol	2722.20		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C517782&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices