(1aR,1a1S,9bS,10S,11R,11aS)-7,8,11-Trimethoxy-1

Inchi: InChI=1S/C18H23NO5/c1-21-11-6-9-8-19-5-4-18-16(19)13(10(9)7-12(11)22-2)14(20)15(
InchiKey: PXSBFPSCQXSITH-UHFFFAOYSA-N
Formula: C18H23NO5
SMILES: COc1cc2c(cc1OC)C1C(O)C(OC)C3OC34CCN(C2)C14
Mol. weight [g/mol]: 333.38
CAS: 145237-00-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	0.902		Crippen Method
mcvol	236.610	ml/mol	McGowan Method
rinpol	2756.70		NIST Webbook
rinpol	2756.70		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C145237009&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/99-445-9/1aR-1a1S-9bS-10S-11R-11aS-7-8-11-Trimethoxy-1a1-2-3-5-9b-10-11-11a-oc