(R)-1-Methoxy-6-methyl-5,6,6a,7-tetrahydro-4H-di

Inchi: InChI=1S/C18H19NO2/c1-19-8-7-12-10-15(20)18(21-2)17-13-6-4-3-5-11(13)9-14(19)16(
InchiKey: AKXOIHNFHOEPHN-CQSZACIVSA-N
Formula: C18H19NO2
SMILES: COc1c(O)cc2c3c1-c1ccccc1CC3N(C)CC2
Mol. weight [g/mol]: 281.35
CAS: 3153-55-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	3.153		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
rinpol	2447.10		NIST Webbook
rinpol	2447.10		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=C3153557&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