(+)-Roemerine

Other names: (R)-7-Methyl-6,7,7a,8-tetrahydro-5H-[1,3]dioxolo[4',5':4,5]benzo[1,2,3-de]benzo[g]quinolin
Inchi: InChI=1S/C18H17NO2/c1-19-7-6-12-9-15-18(21-10-20-15)17-13-5-3-2-4-11(13)8-14(19)
InchiKey: JCTYWRARKVGOBK-CQSZACIVSA-N
Formula: C18H17NO2
SMILES: CN1CCc2cc3c(c4c2C1Cc1ccccc1-4)OCO3
Mol. weight [g/mol]: 279.33
CAS: 548-08-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	3.167		Crippen Method
mcvol	206.100	ml/mol	McGowan Method
rinpol	2575.20		NIST Webbook
rinpol	2575.20		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C548083&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

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