

Cytidine, N-methyl-, 2',3',5'-trimethyl ether

Inchi: InChI=1S/C13H21N3O5/c1-14-9-5-6-16(13(17)15-9)12-11(20-4)10(19-3)8(21-12)7-18-2/
InchiKey: TXQNLIBYRUTPK-UHFFFAOYSA-N
Formula: C13H21N3O5
SMILES: CNc1ccn(C2OC(COC)C(OC)C2OC)c(=O)n1
Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.48		Crippen Method
logp	-0.141		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
rinpola	2275.80		NIST Webbook
rinpola	2275.80		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U332729&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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