9-[(1,3-dihydroxy-2-propoxy)methyl] guanine

Other names: 9-[(1,3-dihydroxy-2-propoxy)methyl]guanine
Inchi: InChI=1S/C9H13N5O4/c10-9-12-7-6(8(17)13-9)11-3-14(7)4-18-5(1-15)2-16/h3,5,15-16H
InchiKey: IRSCQMHQWWYFCW-UHFFFAOYSA-N
Formula: C9H13N5O4
SMILES: Nc1nc(=O)c2ncn(COC(CO)CO)c2[nH]1
Mol. weight [g/mol]: 255.23

Physical Properties

Property code	Value	Unit	Source
logp	-2.453		Crippen Method
mcvol	172.130	ml/mol	McGowan Method

Sources

Effect of Solvent Properties and Composition on the Solubility of Ganciclovir Form I:	https://www.doi.org/10.1021/acs.jced.8b01080
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume