

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 Macrolide Antibiotics

<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.cheméo.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

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<https://www.cheméo.com/cid/108-721-1/9-1-3-dihydroxy-2-propoxy-methyl-guanine.pdf>

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