

6-Methylmercaptopurine riboside

Inchi:	InChI=1S/C11H14N4O4S/c1-20-10-6-9(12-3-13-10)15(4-14-6)11-8(18)7(17)5(2-16)19-11
InchiKey:	ZDRFDHHANOYUTE-UHFFFAOYSA-N
Formula:	C11H14N4O4S
SMILES:	CSc1ncnc2c1ncn2C1OC(CO)C(O)C1O
Mol. weight [g/mol]:	298.32
CAS:	342-69-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Cheméo Relay (1.0)
logp	-0.840		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
tf	437.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.cheméo.com/cid/111-571-4/6-Methylmercaptopurine-riboside.pdf>

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