

5-Methyluridine

Other names:	1-«beta»-D-Ribofuranosylthymine «beta»-D-Ribofuranoside, thymine-1 «beta»-D-Ribofuranosylthymine Ribosylthymine Ribothymidine Thymine ribofuranoside Thymine riboside 2,4(1H,3H)-Pyrimidinedione, 5-methyl-1-«beta»-D-ribofuranosyl- 5-Methyluridine
Inchi:	InChI=1S/C10H14N2O6/c1-4-2-12(10(17)11-8(4)16)9-7(15)6(14)5(3-13)18-9/h2,5-7,9,13
InchiKey:	DWRXFEITVBNRMK-UHFFFAOYSA-N
Formula:	C10H14N2O6
SMILES:	Cc1cn(C2OC(CO)C(O)C2O)c(=O)[nH]c1=O
Mol. weight [g/mol]:	258.23

Physical Properties

Property code	Value	Unit	Source
affp	908.80	kJ/mol	NIST Webbook
logp	-3.025		Crippen Method
mcvol	172.320	ml/mol	McGowan Method
tf	453.86	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1463101&Units=SI>

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):

Legend

affp:	Proton affinity
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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