

(-)-(5)-Bromouridine

Other names:	Uridine, 5-bromo- 5-Bromouracil ribonucleoside 1-«beta»-Ribofuranosyl-5-bromo-uracil 5-Bromouridine
Inchi:	InChI=1S/C9H11BrN2O6/c10-3-1-12(9(17)11-7(3)16)8-6(15)5(14)4(2-13)18-8/h1,4-6,8,1
InchiKey:	AGFIRQJZCNVMCW-UHFFFAOYSA-N
Formula:	C9H11BrN2O6
SMILES:	O=c1[nH]c(=O)n(C2OC(CO)C(O)C2O)cc1Br
Mol. weight [g/mol]:	323.10
CAS:	957-75-5

Physical Properties

Property code	Value	Unit	Source
log10ws	0.22		Crippen Method
logp	-2.571		Crippen Method
mcvol	175.730	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C957755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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