6-MERCAPTOPURINE RIBOSIDE

Other names:	6-MP-Riboside
	6-MPR
	6-Mercapto-9«beta»-D-ribofuranosyl-9H-purine
	6-Mercaptoinosine
	6-Mercaptopurine 9«beta»-D-ribofuranoside
	6-Mercaptopurine ribonucleoside
	6-Mercaptopurine riboside
	6-Thioinosine
	6-Thiopurine ribonucleoside
	6-Thiopurine riboside
	6H-Purine-6-thione, 1,9-dihydro-9-«beta»-D-ribofuranosyl-
	9-«beta»-D-Ribofuranosyl-9H-purine-6-thiol
	9H-Purine-6(1H)-thione, 9-«beta»-D-ribofuranosyl-
	9H-Purine-6-thiol, 9-«beta»-D-ribofuranosyl-
	9H-Purine-6-thiol, 9-«beta»-D-ribofuransoyl-
	9H-purine-6-thiol, 9-beta-d-ribofuranosyl- (keto form)
	Inosine, 6-thio-
	NSC 4911
	Ribosyl-6-thiopurine
	Thionosine
	Tioinosine
Inchi:	InChI=1S/C10H12N4O4S/c15-1-4-6(16)7(17)10(18-4)14-3-13-5-8(14)11-2-12-9(5)19/h2-
InchiKey:	NKGPJODWTZCHGF-UHFFFAOYSA-N
Formula:	C10H12N4O4S
SMILES:	OCC1OC(n2cnc3c(S)ncnc32)C(O)C1O
Mol. weight [g/mol]:	284.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Cheméo Relay (1.0)
logp	-1.274		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
tf	469.36	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C574254&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

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