

9H-purine-6(1h)-thione, 1-methyl-9-beta-d-ribofuranosyl-

Inchi:	InChI=1S/C11H14N4O4S/c1-14-3-13-9-6(11(14)20)12-4-15(9)10-8(18)7(17)5(2-16)19-10
InchiKey:	KAFKQYRSRIAGNP-NCYAXNGYSA-N
Formula:	C11H14N4O4S
SMILES:	Cn1cnc2c(ncn2C2OC(CO)C(O)C2O)c1=S
Mol. weight [g/mol]:	298.32
CAS:	26001-41-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	-0.889		Crippen Method
mcvol	195.820	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26001412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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