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