

2-Propanone, [(9-beta-d-ribofuranosyl-9h-purin-6-yl)thio]-

Inchi:	InChI=1S/C13H16N4O5S/c1-6(19)3-23-12-8-11(14-4-15-12)17(5-16-8)13-10(21)9(20)7(2
InchiKey:	YFMRPNGBHLFTOL-UHFFFAOYSA-N
Formula:	C13H16N4O5S
SMILES:	CC(=O)CSc1ncnc2c1ncn2C1OC(CO)C(O)C1O
Mol. weight [g/mol]:	340.36
CAS:	71052-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	-0.881		Crippen Method
mcvol	225.570	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=C71052749&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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