

9H-purine-6-thiol, 2-fluoro-9-beta-d-ribofuranosyl-

Inchi:	InChI=1S/C10H11FN4O4S/c11-10-13-7-4(8(20)14-10)12-2-15(7)9-6(18)5(17)3(1-16)19-9
InchiKey:	MORQXRUBNWQJJH-UHFFFAOYSA-N
Formula:	C10H11FN4O4S
SMILES:	OCC1OC(n2cnc3c(S)nc(F)nc32)C(O)C1O
Mol. weight [g/mol]:	302.28
CAS:	792-16-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	-1.134		Crippen Method
mcvol	183.500	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C792165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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