9H-purine-6(1h)-thione, 9-beta-d-ribofuranosyl-, 3',5'-cyclic phosphate

Inchi:	InChI=1S/C10H11N4O6PS/c15-6-7-4(1-18-21(16,17)20-7)19-10(6)14-3-13-5-8(14)11-2-1
InchiKey:	JTFLPNUVMQRDAX-UHFFFAOYSA-N
Formula:	C10H11N4O6PS
SMILES:	O=P1(O)OCC2OC(n3cnc4c(=S)[nH]cnc43)C(O)C2O1
Mol. weight [g/mol]:	346.26
CAS:	20096-88-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	-0.219		Crippen Method
mcvol	203.070	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20096882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:
https://www.chemeo.com/cid/75-614-7/9H-purine-6-1h-thione-9-beta-d-ribofuranosyl-3-5-cyclic-phosphate.pdf
Generated by Cheméo on 2024-10-12 02:41:17.313421564 +0000 UTC m=+3281739.950390812.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.