

9H-purine-6(1h)-thione, 2,9-diethyl-

Inchi:	InChI=1S/C9H12N4S/c1-3-6-11-8-7(9(14)12-6)10-5-13(8)4-2/h5H,3-4H2,1-2H3,(H,11,12)
InchiKey:	AHPPXBAAWSUBA-UHFFFAOYSA-N
Formula:	C9H12N4S
SMILES:	CCc1nc2c(ncn2CC)c(=S)[nH]1
Mol. weight [g/mol]:	208.28
CAS:	6223-60-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	1.589		Crippen Method
mcvol	155.020	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=C6223605&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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