

Purine, 6-dimethylamino-2-methylthio-

Inchi:	InChI=1S/C8H11N5S/c1-13(2)7-5-6(10-4-9-5)11-8(12-7)14-3/h4H,1-3H3,(H,9,10,11,12)
InchiKey:	XTAILPVSOIQFHP-UHFFFAOYSA-N
Formula:	C8H11N5S
SMILES:	CSc1nc(N(C)C)c2[nH]cnc2n1
Mol. weight [g/mol]:	209.27
CAS:	1681-11-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	0.659		Crippen Method
mcvol	150.910	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1681114&Units=SI

Legend

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

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<https://www.chemeo.com/cid/61-765-5/Purine-6-dimethylamino-2-methylthio.pdf>

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