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