

9H-Purin-6-amine,N,9-dimethyl-

Other names:	6-Methylamino-9-methyl purine
Inchi:	InChI=1S/C7H9N5/c1-8-6-5-7(10-3-9-6)12(2)4-11-5/h3-4H,1-2H3,(H,8,9,10)
InchiKey:	GRDLXXJSRHDATN-UHFFFAOYSA-N
Formula:	C7H9N5
SMILES:	CNc1ncnc2c1ncn2C
Mol. weight [g/mol]:	163.18
CAS:	2009-52-1

Physical Properties

Property code	Value	Unit	Source
ie	7.95	eV	NIST Webbook
log10ws	-3.87		Crippen Method
logp	0.405		Crippen Method
mcpvol	120.470	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	115.50 ± 1.70	kJ/mol	352.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2009521&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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