1H-Purin-6-amine, N,N-dimethyl-

Other names:	Adenine, N,N-dimethyl- 6-(Dimethylamino)purine N(6),N(6)-Dimethyladenine N,N-Dimethyladenine 6-Dimethyladenine Dimethyladenine N,N-Dimethyl-6-aminopurine Purine, 6-(dimethylamino)- Adenine, N6,N6-dimethyl- 6-Dimethylamino-9H-purine NSC 401568 Dimethylaminopurine
Inchi:	InChI=1S/C7H9N5/c1-12(2)7-5-6(9-3-8-5)10-4-11-7/h3-4H,1-2H3,(H,8,9,10,11)
InchiKey:	BVIAOQMSVZHOJM-UHFFFAOYSA-N
Formula:	C7H9N5
SMILES:	CN(C)c1ncnc2[nH]cnc12
Mol. weight [g/mol]:	163.18
CAS:	938-55-6

Physical Properties

Property code	Value	Unit	Source
ie	7.78	eV	NIST Webbook
log10ws	-1.70		Crippen Method
logp	-0.063		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1804.00		NIST Webbook
rinpol	1878.20		NIST Webbook
rinpol	1878.20		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	115.50 ± 2.10	kJ/mol	394.00	NIST Webbook

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=C938556&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
rinpol:	Non-polar retention indices