9H-PURIN-6-AMINE, N,N,9-TRIMETHYL-

Other names: N,N,9-trimethyladenine
Inchi: InChI=1S/C8H11N5/c1-12(2)7-6-8(10-4-9-7)13(3)5-11-6/h4-5H,1-3H3
InchiKey: GQKLJZOIXKFFQC-UHFFFAOYSA-N
Formula: C8H11N5
SMILES: CN(C)c1ncnc2c1ncn2C
Mol. weight [g/mol]: 177.21

Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	Cheméo Relay (1.0)
log10ws	-1.85		Cheméo Relay (1.0)
logp	0.429		Crippen Method
mcvol	134.560	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	101.70 ± 2.10	kJ/mol	334.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3013829&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

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