

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
CAS:	3013-82-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	0.429		Crippen Method
mcpvol	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3013829&Units=SI
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

Legend

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

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