

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

Other names:	Adenine, N-methyl- N6-Methyladenine 6-(Methylamino)purine 6-Methyladenine 6-Monomethylaminopurine 6-MAP N6-Monomethyladenine NSC 11580 6-(N-Methylamino)purine methyl(purin-6-yl)amine
Inchi:	InChI=1S/C6H7N5/c1-7-5-4-6(10-2-8-4)11-3-9-5/h2-3H,1H3,(H2,7,8,9,10,11)
InchiKey:	CKOMXBHMKXXTNW-UHFFFAOYSA-N
Formula:	C6H7N5
SMILES:	CNc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	149.15
CAS:	443-72-1

Physical Properties

Property code	Value	Unit	Source
ie	8.15	eV	NIST Webbook
ie	8.15	eV	NIST Webbook
ie	8.39	eV	NIST Webbook
log10ws	-1.80		Crippen Method
logp	-0.087		Crippen Method
mcpvol	106.380	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	123.00 ± 21.00	kJ/mol	410.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C443721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/58-026-9/1H-Purin-6-amine-N-methyl.pdf>

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