

6H-Purin-6-one, 2-amino-1,7-dihydro-7-methyl-

Other names:	2-Amino-1,7-dihydro-7-methyl-6H-purin-6-one 2-Amino-7-methyl-1,7-dihydro-6H-purin-6-one 2-Amino-7-methylhypoxanthine 6H-Purin-6-one, 2-amino-1,7-dihydro-7-methyl- Guanine, 7-methyl- N7-Methylguanine NSC 193444
Inchi:	InChI=1S/C6H7N5O/c1-11-2-8-4-3(11)5(12)10-6(7)9-4/h2H,1H3,(H3,7,9,10,12)
InchiKey:	FZWGECJQACGGTI-UHFFFAOYSA-N
Formula:	C6H7N5O
SMILES:	Cn1cnc2nc(N)[nH]c(=O)c21
Mol. weight [g/mol]:	165.16

Physical Properties

Property code	Value	Unit	Source
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-2.13		Cheméo Relay (1.0)
logp	-1.243		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
tf	609.58	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C578767&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):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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