1H-Purine, 6-methyl-

Other names:	Purine, 6-methyl- 6-Methylpurine 6-Methyl-1H-purine
Inchi:	InChI=1S/C6H6N4/c1-4-5-6(9-2-7-4)10-3-8-5/h2-3H,1H3,(H,7,8,9,10)
InchiKey:	SYMHUEFSSMBHJA-UHFFFAOYSA-N
Formula:	C6H6N4
SMILES:	Cc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	134.14
CAS:	2004-03-7

Physical Properties

Property code	Value	Unit	Source
affp	939.20	kJ/mol	NIST Webbook
basg	907.30	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-2.27		Crippen Method
logp	0.179		Crippen Method
mcvol	96.400	ml/mol	McGowan Method

Sources

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=C2004037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity

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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