1H-Imidazole-4-ethanamine, N,N-dimethyl-

Other names:	N,N-Dimethylhistamine
	Imidazole, 4-[2-(dimethylamino)ethyl]-
	N«alpha»,N«alpha»-Dimethylhistamine
	N«omega»,N«omega»-Dimethylhistamine
	N',N'-Dimethylhistamine
	4-(2-Dimethylaminoethyl)imidazole
	N-alpha,N-alpha-Dimethylhistamine
	N-omega,N-omega-Dimethylhistamine
	SU-416
Inchi:	InChI=1S/C7H13N3/c1-10(2)4-3-7-5-8-6-9-7/h5-6H,3-4H2,1-2H3,(H,8,9)
InchiKey:	ZJDIMSMQXMWMCF-UHFFFAOYSA-N
Formula:	C7H13N3
SMILES:	CN(C)CCc1c[nH]cn1
Mol. weight [g/mol]:	139.20
CAS:	673-46-1

Physical Properties

Property code	Value	Unit	Source
affp	1022.00	kJ/mol	NIST Webbook
basg	990.10	kJ/mol	NIST Webbook
log10ws	-0.67		Crippen Method
logp	0.032		Crippen Method
mcvol	119.970	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C673461&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume