

1H-Imidazole, 1,4-dimethyl-

Other names:	1,4-Dimethylimidazole
Inchi:	InChI=1S/C5H8N2/c1-5-3-7(2)4-6-5/h3-4H,1-2H3
InchiKey:	BLHTXORQJNCSII-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	Cc1cn(C)cn1
Mol. weight [g/mol]:	96.13
CAS:	6338-45-0

Physical Properties

Property code	Value	Unit	Source
affp	976.70	kJ/mol	NIST Webbook
basg	944.90	kJ/mol	NIST Webbook
log10ws	-3.00		Crippen Method
logp	0.729		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	979.00		NIST Webbook
rinpol	979.00		NIST Webbook
ripol	1677.00		NIST Webbook
ripol	1677.00		NIST Webbook
tb	472.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6338450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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