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/ci990307l
Crippen Method: https://www.chemeo.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