

1H-Imidazole-4-methanol, 5-methyl-

Other names:	Imidazole-4-methanol, 5-methyl- 4-Methylimidazole-5-methanol Imidazole, 4-methyl-5-hydroxymethyl- 5-methyl-1H-imidazole-4-methanol
Inchi:	InChI=1S/C5H8N2O/c1-4-5(2-8)7-3-6-4/h3,8H,2H2,1H3,(H,6,7)
InchiKey:	AXJZCJSXNZZMDU-UHFFFAOYSA-N
Formula:	C5H8N2O
SMILES:	Cc1nc[nH]c1CO
Mol. weight [g/mol]:	112.13
CAS:	29636-87-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	-0.271		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
rinpola	955.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29636871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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