

5-Chloro-1-methylimidazole

Other names:	1H-Imidazole, 5-chloro-1-methyl- 5-chloro-1-methyl-1H-imidazole
Inchi:	InChI=1S/C4H5ClN2/c1-7-3-6-2-4(7)5/h2-3H,1H3
InchiKey:	NYDGOZPYEABERA-UHFFFAOYSA-N
Formula:	C4H5ClN2
SMILES:	Cn1cncc1Cl
Mol. weight [g/mol]:	116.55
CAS:	872-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	1.073		Crippen Method
mvol	79.960	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.50 ± 0.50	K	1.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C872491&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tbrp:	Boiling point at reduced pressure

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