

5-Chloro-1,3-dimethylpyrazole

Other names:	1H-Pyrazole, 5-chloro-1,3-dimethyl-
Inchi:	InChI=1S/C5H7ClN2/c1-4-3-5(6)8(2)7-4/h3H,1-2H3
InchiKey:	DDUSLFAWARYAPR-UHFFFAOYSA-N
Formula:	C5H7ClN2
SMILES:	Cc1cc(Cl)n(C)n1
Mol. weight [g/mol]:	130.57
CAS:	54454-10-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	1.382		Crippen Method
mcvol	94.050	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C54454103&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/56-309-7/5-Chloro-1-3-dimethylpyrazole.pdf>

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