

4,5-Dichloroimidazole

Inchi:	InChI=1S/C3H2Cl2N2/c4-2-1-6-7-3(2)5/h1H,(H,6,7)
InchiKey:	CHUPRLGXGZETTE-UHFFFAOYSA-N
Formula:	C3H2Cl2N2
SMILES:	Clc1c[nH]nc1Cl
Mol. weight [g/mol]:	136.97
CAS:	15965-30-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	1.235		Crippen Method
mcvol	78.110	ml/mol	McGowan Method

Sources

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=C15965307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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