

C5H4Cl2N2

Inchi:	InChI=1S/C5H4Cl2N2/c6-4-1-3(8)2-5(7)9-4/h1-2H,(H2,8,9)
InchiKey:	WAEZOSSWRXDWAX-UHFFFAOYSA-N
Formula:	C5H4Cl2N2
SMILES:	Nc1cc(Cl)nc(Cl)c1
Mol. weight [g/mol]:	163.00
CAS:	2587-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.971		Crippen Method
mcvol	101.990	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2587022&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

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<https://www.chemeo.com/cid/113-690-0/C5H4Cl2N2.pdf>

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