

1H-Pyrazole, 4-chloro-

Other names:	Pyrazole, 4-chloro- 4-Chloropyrazole L-21842
Inchi:	InChI=1S/C3H3ClN2/c4-3-1-5-6-2-3/h1-2H,(H,5,6)
InchiKey:	BADSZRMNXWLUKO-UHFFFAOYSA-N
Formula:	C3H3ClN2
SMILES:	Clc1cn[nH]c1
Mol. weight [g/mol]:	102.52
CAS:	15878-00-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Crippen Method
logp	0.581		Crippen Method
mcvol	65.870	ml/mol	McGowan Method
rinpol	867.00		NIST Webbook
rinpol	867.00		NIST Webbook

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=C15878009&Units=SI

Legend

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

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