

6-Chloroindole

Other names:	1H-Indole, 6-chloro- 6-chloro-1H-indole
Inchi:	InChI=1S/C8H6ClN/c9-7-2-1-6-3-4-10-8(6)5-7/h1-5,10H
InchiKey:	YTYIMDRWPTUAHP-UHFFFAOYSA-N
Formula:	C8H6ClN
SMILES:	Clc1ccc2cc[nH]c2c1
Mol. weight [g/mol]:	151.59
CAS:	17422-33-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.339		Crippen Method
mcvol	106.880	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=C17422332&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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