

1H-Indole, 5-chloro-

Other names:	5-Chloroindole 5-Chloro-1H-indole Indole, 5-chloro-
Inchi:	InChI=1S/C8H6ClN/c9-7-1-2-8-6(5-7)3-4-10-8/h1-5,10H
InchiKey:	MYTGFBZJLDLWQG-UHFFFAOYSA-N
Formula:	C8H6ClN
SMILES:	Clc1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	151.59
CAS:	17422-32-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.339		Crippen Method
mcvol	106.880	ml/mol	McGowan Method
rinpol	1361.00		NIST Webbook
rinpol	1361.00		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=C17422321&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

Latest version available from:

<https://www.cheméo.com/cid/81-332-3/1H-Indole-5-chloro.pdf>

Generated by Cheméo on 2024-04-25 18:38:27.441992385 +0000 UTC m=+16359556.362569700.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.