

1H-Indole, 4-chloro-

Other names:	4-Chloroindole Indole, 4-chloro-
Inchi:	InChI=1S/C8H6ClN/c9-7-2-1-3-8-6(7)4-5-10-8/h1-5,10H
InchiKey:	SVLZRRCRXNHITBY-UHFFFAOYSA-N
Formula:	C8H6ClN
SMILES:	Clc1cccc2[nH]ccc12
Mol. weight [g/mol]:	151.59
CAS:	25235-85-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.339		Crippen Method
mcvol	106.880	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.70	K	0.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25235852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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