

3-chloro-1H-indazole

Inchi:	InChI=1S/C7H5ClN2/c8-7-5-3-1-2-4-6(5)9-10-7/h1-4H,(H,9,10)
InchiKey:	QPHAGNNWDZSKJH-UHFFFAOYSA-N
Formula:	C7H5ClN2
SMILES:	Clc1[nH]nc2ccccc12
Mol. weight [g/mol]:	152.58
CAS:	29110-74-5

Physical Properties

Property code	Value	Unit	Source
ie	8.41	eV	NIST Webbook
log10ws	-2.95		Crippen Method
logp	1.734		Crippen Method
mcvol	102.770	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29110745&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

ie:	Ionization energy
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/112-546-1/3-chloro-1H-indazole.pdf>

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