

3-Indolecarbonitrile

Other names:	Indole-3-carbonitrile 3-Cyanoindole
Inchi:	InChI=1S/C9H6N2/c10-5-7-6-11-9-4-2-1-3-8(7)9/h1-4,6,11H
InchiKey:	CHIFTAQVXHNVRW-UHFFFAOYSA-N
Formula:	C9H6N2
SMILES:	N#Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	142.16
CAS:	5457-28-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	1.558		Crippen Method
mvol	110.110	ml/mol	McGowan Method

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=C5457283&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/18-202-7/3-Indolecarbonitrile.pdf>

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