

1H-Indole-3-acetonitrile

Other names:	Indole-3-acetonitrile Indoleacetonitrile Indolylacetonitrile 3-Indolylacetonitrile Indolyl-3-acetonitrile 3-Indoleacetonitrile «beta»-Indoleacetonitrile Acetonitrile, 3-indolyl- USAF CB-29 3-(Cyanomethyl)indole 3-Indolacetonitrile 3-Cyanomethyl-1H-indole NSC 523272 indol-3-ylacetonitrile
Inchi:	InChI=1S/C10H8N2/c11-6-5-8-7-12-10-4-2-1-3-9(8)10/h1-4,7,12H,5H2
InchiKey:	DMCPFOBLJMLSX-UHFFFAOYSA-N
Formula:	C10H8N2
SMILES:	<chem>N#CCc1c[nH]c2cccc12</chem>
Mol. weight [g/mol]:	156.18
CAS:	771-51-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.16		Crippen Method
logp	1.752		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
rmpol	1814.80		NIST Webbook
rmpol	1740.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.70	K	0.03	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C771517&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
tbrp:	Boiling point at reduced pressure

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