

1H-Indole-3-acetonitrile, 1-(trimethylsilyl)-

Other names:	Indole-3-acetonitrile, TMS Indole-3-acetonitrile, tms derivative
Inchi:	InChI=1S/C13H16N2Si/c1-16(2,3)15-10-11(8-9-14)12-6-4-5-7-13(12)15/h4-7,10H,8H2,1-
InchiKey:	QIPOVLUFFYDMLH-UHFFFAOYSA-N
Formula:	C13H16N2Si
SMILES:	C[Si](C)(C)n1cc(CC#N)c2ccccc21
Mol. weight [g/mol]:	228.37
CAS:	74367-49-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	3.390		Crippen Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-311-1/1H-Indole-3-acetonitrile-1-trimethylsilyl.pdf>

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