

1H-Indole-2-carbonitrile, 3-methyl-

Other names: Indole-2-carbonitrile, 3-methyl-
Inchi: InChI=1S/C10H8N2/c1-7-8-4-2-3-5-9(8)12-10(7)6-11/h2-5,12H,1H3
InchiKey: XOILSNZVQVLOED-UHFFFAOYSA-N
Formula: C10H8N2
SMILES: Cc1c(C#N)[nH]c2ccccc12
Mol. weight [g/mol]: 156.18
CAS: 13006-59-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	1.866		Crippen Method
mcvol	124.200	ml/mol	McGowan Method
rinpola	1463.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13006592&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
rinpola: Non-polar retention indices

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