

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

Other names: 1-Methyl-2,3-dihydro-1H-indole
Inchi: InChI=1S/C9H11N/c1-10-7-6-8-4-2-3-5-9(8)10/h2-5H,6-7H2,1H3
InchiKey: FIRXFHJQGIIJDB-UHFFFAOYSA-N
Formula: C9H11N
SMILES: CN1CCc2ccccc21
Mol. weight [g/mol]: 133.19
CAS: 824-21-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	1.679		Crippen Method
mcvol	113.030	ml/mol	McGowan Method
rinpol	1248.00		NIST Webbook
rinpol	1230.00		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1756.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C824215&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

ripol: Polar retention indices

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