

N-ethyl-dihydroindole

Inchi: InChI=1S/C10H13N/c1-2-11-8-7-9-5-3-4-6-10(9)11/h3-6H,2,7-8H2,1H3
InchiKey: JJFUPPZOYYMAFC-UHFFFAOYSA-N
Formula: C10H13N
SMILES: CCN1CCc2ccccc21
Mol. weight [g/mol]: 147.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Crippen Method
logp	2.069		Crippen Method
mcvol	127.120	ml/mol	McGowan Method
rinpol	1305.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1322.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1844.00		NIST Webbook
ripol	1830.00		NIST Webbook

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=R135325&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

ripol: Polar retention indices

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