

N-ethyl-Octahydroindole

Inchi: InChI=1S/C10H19N/c1-2-11-8-7-9-5-3-4-6-10(9)11/h9-10H,2-8H2,1H3
InchiKey: GSXWVOZWKACRTO-UHFFFAOYSA-N
Formula: C10H19N
SMILES: CCN1CCC2CCCCC21
Mol. weight [g/mol]: 153.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	2.271		Crippen Method
mcvol	140.020	ml/mol	McGowan Method
ripol	1202.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1394.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R135330&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
ripol: Non-polar retention indices
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/59-289-7/N-ethyl-Octahydroindole.pdf>

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