4H-Pyrrolo[3,2,1-ij]quinoline, 1,2,5,6-tetrahydro-6-methyl-

Other names: 6-Methyllilolidine
Inchi: InChI=1S/C12H15N/c1-9-5-7-13-8-6-10-3-2-4-11(9)12(10)13/h2-4,9H,5-8H2,1H3
InchiKey: ZVNKPQBRBWFFON-UHFFFAOYSA-N
Formula: C12H15N
SMILES: CC1CCN2CCc3cccc1c32
Mol. weight [g/mol]: 173.25
CAS: 40135-93-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	2.556		Crippen Method
mcvol	144.440	ml/mol	McGowan Method
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40135931&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

Latest version available from: