

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

Other names:	6-Methylilolidine
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

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