Julolidine

Other names:	1H,5H-Benzo[ij]quinolizine, 2,3,6,7-tetrahydro-
	2,3,6,7-Tetrahydro-1H,5H-benzo(ij)quinolizine
Inchi:	InChI=1S/C12H15N/c1-4-10-6-2-8-13-9-3-7-11(5-1)12(10)13/h1,4-5H,2-3,6-9H2
InchiKey:	DZFWNZJKBJOGFQ-UHFFFAOYSA-N
Formula:	C12H15N
SMILES:	c1cc2c3c(c1)CCCN3CCC2
Mol. weight [g/mol]:	173.25
CAS:	479-59-4

Physical Properties

Property code	Value	Unit	Source
ie	6.65 ± 0.02	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.385		Crippen Method
mcvol	144.440	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C479594&Units=SI
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

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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