5-acetyl-2,3-1H-pyrrolizine

Other names:	5-acetyl-2,3-dihydro-1H-pyrrolizine
	5-acetyl-2,3-dihydro-lH-pyrrolizine
Inchi:	InChI=1S/C9H11NO/c1-7(11)9-5-4-8-3-2-6-10(8)9/h4-5H,2-3,6H2,1H3
InchiKey:	NWSCEJHRUVCUSX-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CC(=O)c1ccc2n1CCC2
Mol. weight [g/mol]:	149.19
CAS:	55041-85-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	1.637		Crippen Method
mcvol	118.900	ml/mol	McGowan Method
rinpol	1335.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1354.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2021.00		NIST Webbook
ripol	2021.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55041855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices