7-acetyl-5-methyl-2,3-dihydro-(1H)-pyrrolizine

Other names: 7-Acetyl-5-methy1-2,3-dihydro-1H-pyrrolizine
Inchi: InChI=1S/C10H13NO/c1-7-6-9(8(2)12)10-4-3-5-11(7)10/h6H,3-5H2,1-2H3
InchiKey: DJAGDEJXGVMMGJ-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CC(=O)c1cc(C)n2c1CCC2
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	1.945		Crippen Method
mcvol	132.990	ml/mol	McGowan Method
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R231111&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

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices