5-acetyl-6-methyl-2,3-dihydro-1H-pyrrolizine

Inchi: InChI=1S/C10H13NO/c1-7-6-9-4-3-5-11(9)10(7)8(2)12/h6H,3-5H2,1-2H3
InchiKey: FEOYYZKCVVLICI-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CC(=O)c1c(C)cc2n1CCC2
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
ripol	2187.00		NIST Webbook
ripol	2187.00		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=R220963&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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