5-Propionyl-7-methyl-2,3-dihydro-1H-pyrrolizine

Inchi: InChI=1S/C11H15NO/c1-3-11(13)10-7-8(2)9-5-4-6-12(9)10/h7H,3-6H2,1-2H3
InchiKey: COEUIAKZDWIIQD-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CCC(=O)c1cc(C)c2n1CCC2
Mol. weight [g/mol]: 177.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.335		Crippen Method
mcvol	147.080	ml/mol	McGowan Method
ripol	2139.00		NIST Webbook

Sources

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=R312082&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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