5-propionyl-2,3-dihydro-1H-pyrrolizine

Inchi: InChI=1S/C10H13NO/c1-2-10(12)9-6-5-8-4-3-7-11(8)9/h5-6H,2-4,7H2,1H3
InchiKey: WOCOJSXECLIQIX-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CCC(=O)c1ccc2n1CCC2
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	2.027		Crippen Method
mcvol	132.990	ml/mol	McGowan Method
rinpol	1452.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1452.00		NIST Webbook
rinpol	1468.00		NIST Webbook
ripol	2091.00		NIST Webbook
ripol	2091.00		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=R220958&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
rinpol: Non-polar retention indices

ripol: Polar retention indices