5-formyl-6-methyl-2,3-dihydro-(1H)-pyrrolizine

Inchi: InChI=1S/C9H11NO/c1-7-5-8-3-2-4-10(8)9(7)6-11/h5-6H,2-4H2,1H3
InchiKey: NWFQKPJYEJRQRI-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: Cc1cc2n(c1C=O)CCC2
Mol. weight [g/mol]: 149.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.555		Crippen Method
mcvol	118.900	ml/mol	McGowan Method
rinpol	1484.00		NIST Webbook
ripol	2157.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R231077&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

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