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

Inchi: InChI=1S/C8H9NO/c10-6-8-4-3-7-2-1-5-9(7)8/h3-4,6H,1-2,5H2
InchiKey: XDRGCZAFSAFSLR-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: O=Cc1ccc2n1CCC2
Mol. weight [g/mol]: 135.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	1.247		Crippen Method
mcvol	104.810	ml/mol	McGowan Method
ripol	1993.00		NIST Webbook
ripol	1993.00		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=R182846&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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