

5-(3-hydroxypropionyl)-2,3-dihydro-1H-pyrrolizine

Inchi:	InChI=1S/C10H13NO2/c12-7-5-10(13)9-4-3-8-2-1-6-11(8)9/h3-4,12H,1-2,5-7H2
InchiKey:	DLLQYHQNPSCSK-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	O=C(CCO)c1ccc2n1CCC2
Mol. weight [g/mol]:	179.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	0.999		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
rinsol	1723.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R225151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/94-370-7/5-3-hydroxypropionyl-2-3-dihydro-1H-pyrrolizine.pdf>

Generated by Cheméo on 2024-04-23 15:40:36.980624045 +0000 UTC m=+16176085.901201357.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.