

1H-Pyrrolizine-1-carboxylic acid, hexahydro-, methyl ester

Other names: Chysin A
Inchi: InChI=1S/C9H15NO2/c1-12-9(11)7-4-6-10-5-2-3-8(7)10/h7-8H,2-6H2,1H3
InchiKey: CFWZLIYRMYFCIH-UHFFFAOYSA-N
Formula: C9H15NO2
SMILES: COC(=O)C1CCN2CCCC12
Mol. weight [g/mol]: 169.22
CAS: 54514-96-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	0.644		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
rinsol	1283.00		NIST Webbook
rinsol	1283.00		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=C54514964&Units=SI>

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/97-107-6/1H-Pyrrolizine-1-carboxylic-acid-hexahydro-methyl-ester.pdf>

Generated by Cheméo on 2024-05-04 04:49:01.692149177 +0000 UTC m=+17087390.612726488.

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