

Chlorocarbene artifact of 7«alpha»-Hydroxy-1-methoxymethyl-8«alpha»-pyrrolizidine

Inchi: InChI=1S/C9H14ClNO/c10-7-5-9(7)2-4-11-3-1-6(12)8(9)11/h6-8,12H,1-5H2/t6-,7?,8?,9?/
InchiKey: RWJHSCSVXJXWHL-JUGFDQIVSA-N
Formula: C9H14ClNO
SMILES: OC1CCN2CCC3(CC3Cl)C12
Mol. weight [g/mol]: 187.67

Physical Properties

Property code	Value	Unit	Source
logp	0.823		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
rinpol	1637.00		NIST Webbook
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Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R590242&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/98-831-1/Chlorocarbene-artifact-of-7-alpha-Hydroxy-1-methoxymethyl-8-alpha-pyrrolizidine>

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