Chlorocarbene aftifact of 7«beta»-Hydroxy-1-methylene-8«alpha»/«beta»-py

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	1426.00		NIST Webbook
rinpol	1426.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R590237&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.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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