7«alpha»-Angeloyl-1-chloromethyl-1,2-dehydropy

Inchi: InChI=1S/C13H18ClNO2/c1-3-9(2)13(16)17-11-5-7-15-6-4-10(8-14)12(11)15/h3-4,11-12
InchiKey: QPMBQTBGLNEAQX-XLFQXWAYSA-N
Formula: C13H18ClNO2
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(CCl)C12
Mol. weight [g/mol]: 255.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	2.118		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299528&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
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.