7-Angeloyl-1-formyl-6,7-dihydro-5H-pyrrolizine

Inchi: InChI=1S/C13H15NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h3-4,6,8,11H,
InchiKey: LJHFLAIWOBXLFA-OQFOIZHKSA-N
Formula: C13H15NO3
SMILES: CC=C(C)C(=O)OC1CCn2ccc(C=O)c21
Mol. weight [g/mol]: 233.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	2.255		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299637&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