9-(Butyryl-2-ene) supinidine

Inchi: InChI=1S/C12H17NO2/c1-2-4-12(14)15-9-10-6-8-13-7-3-5-11(10)13/h2,4,6,11H,3,5,7-9H
InchiKey: KTHGVVZUCVCGKR-JRBALWBOSA-N
Formula: C12H17NO2
SMILES: CC=CC(=O)OCC1=CCN2CCCC12
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	1.510		Crippen Method
mcvol	167.040	ml/mol	McGowan Method
rinpol	1674.00		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=R240556&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices