Supinidine, 1.beta.,2.beta.-epoxy-O1-methyl-

Other names: Supinidine, 1«beta»,2«beta»-epoxy-O1-methyl-
Inchi: InChI=1S/C9H15NO2/c1-11-6-9-7-3-2-4-10(7)5-8(9)12-9/h7-8H,2-6H2,1H3
InchiKey: KLYKJOPFNDDFNE-UHFFFAOYSA-N
Formula: C9H15NO2
SMILES: COCC12OC1CN1CCCC12
Mol. weight [g/mol]: 169.22

Physical Properties

Property code	Value	Unit	Source
logp	0.248		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
rinpol	1313.00		NIST Webbook
rinpol	1313.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15211082&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices