

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
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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

Latest version available from:

<https://www.chemeo.com/cid/57-047-7/Supinidine-1-beta-2-beta-epoxy-O1-methyl.pdf>

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