

1 «beta»,2 «beta»-Epoxy-1 «alpha»-methoxymethyl-

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
CAS: 15211-08-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.35		Crippen Method
logp	0.248		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
rinsol	1313.00		NIST Webbook
rinsol	1313.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15211082&Units=SI>
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>

Legend

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

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