3,8a-Dimethyl-5-methylene-5,6,8a,9-tetrahydronap

Inchi: InChI=1S/C15H16O2/c1-9-5-4-6-15(3)7-11-12(10(2)8-17-11)14(16)13(9)15/h4,6,8,13H,1
InchiKey: CPLKMTCUMNMEHL-UHFFFAOYSA-N
Formula: C15H16O2
SMILES: C=C1CC=CC2(C)Cc3occ(C)c3C(=O)C12
Mol. weight [g/mol]: 228.29
CAS: 174657-08-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.67		Crippen Method
logp	3.465		Crippen Method
mcvol	179.870	ml/mol	McGowan Method
rinpol	1777.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C174657080&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
rinpol: Non-polar retention indices

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