

(4aS,8aS)-3,8a-Dimethyl-5-methylene-4,4a,5,6,8a,9

Inchi: InChI=1S/C15H18O/c1-10-5-4-6-15(3)8-14-12(7-13(10)15)11(2)9-16-14/h4,6,9,13H,1,5,7
InchiKey: BZQURGSQMBBPRU-HIFRSBDPSA-N
Formula: C15H18O
SMILES: C=C1CC=CC2(C)Cc3occ(C)c3CC12
Mol. weight [g/mol]: 214.30
CAS: 2221-88-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.81		Crippen Method
logp	3.825		Crippen Method
mcvol	178.300	ml/mol	McGowan Method
rinpol	1653.00		NIST Webbook
rinpol	1651.60		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2170.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2221887&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
ripol: Polar retention indices

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