1,4:5,8-Dimethanonaphthalen-9-ol, 1,4,4a,5,6,7,8,8a-octahydro-, stereoisomer

Other names: 1,4:5,8-Dimethanonaphthalen-9-ol, 1,4,4a,5,6,7,8,8a-octahydro-, anti-endo,exo-Tetracyclo[6.2.1.1(3,6).0(2,7)]dodec-4-ene-11-ol, stereoisomer

Inchi: InChI=1S/C12H16O/c13-12-8-3-4-9(12)11-7-2-1-6(5-7)10(8)11/h1-2,6-13H,3-5H2

InchiKey: NGFZLQIRULRVPV-UHFFFAOYSA-N

Formula: C12H16O

SMILES: [O]C1C2CCC1C1C3C=CC(C3)C21

Mol. weight [g/mol]: 176.25

CAS: 28068-45-3

Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
ie	9.01	eV	NIST Webbook
log10ws	-6.83		Crippen Method
logp	2.264		Crippen Method
mcvol	135.920	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28068453&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume