

# 1,4:5,8-Dimethanonaphthalen-9-ol, decahydro-, stereoisomer

**Inchi:** InChI=1S/C12H18O/c13-12-8-3-4-9(12)11-7-2-1-6(5-7)10(8)11/h6-13H,1-5H2  
**InchiKey:** ZPOMMBHYDITYNL-UHFFFAOYSA-N  
**Formula:** C12H18O  
**SMILES:** [O]C1C2CCC1C1C3CCC(C3)C21  
**Mol. weight [g/mol]:** 178.27  
**CAS:** 36197-16-7

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| ie            | 8.90    | eV     | NIST Webbook   |
| ie            | 9.60    | eV     | NIST Webbook   |
| log10ws       | -6.98   |        | Crippen Method |
| logp          | 2.488   |        | Crippen Method |
| mcvol         | 140.220 | ml/mol | McGowan Method |

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C36197167&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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