

# Davanafuran

**Inchi:** InChI=1S/C13H18O2/c1-4-13(3)8-7-12(15-13)10(2)11-6-5-9-14-11/h4-6,9-10,12H,1,7-8H  
**InchiKey:** WBNXESGNGNWXSU-UHFFFAOYSA-N  
**Formula:** C13H18O2  
**SMILES:** C=CC1(C)CCC(C(C)c2ccco2)O1  
**Mol. weight [g/mol]:** 206.28  
**CAS:** 869379-85-1

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.96   |        | Crippen Method |
| logp          | 3.507   |        | Crippen Method |
| mcvol         | 171.150 | ml/mol | McGowan Method |
| rinpol        | 1418.20 |        | NIST Webbook   |
| rinpol        | 1418.20 |        | NIST Webbook   |

## 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=C869379851&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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