

# (S)-Laudanine

**Inchi:** InChI=1S/C20H25NO4/c1-21-8-7-14-11-19(24-3)20(25-4)12-15(14)16(21)9-13-5-6-18(23)  
**InchiKey:** MPYHGNAJOKCMAQ-MRXNPFEDSA-N  
**Formula:** C20H25NO4  
**SMILES:** COc1ccc(CC2c3cc(OC)c(OC)cc3CCN2C)cc1O  
**Mol. weight [g/mol]:** 343.42  
**CAS:** 3122-95-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.94		Crippen Method
logp	3.190		Crippen Method
mcvol	267.740	ml/mol	McGowan Method
rinpol	2784.80		NIST Webbook
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## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3122950&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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>

## 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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