

# L-Tryptophan, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

**Inchi:** InChI=1S/C22H30N2O6/c1-6-28-21(26)23-18(20(25)30-15(5)14(3)4)12-16-13-24(22(27)28)29  
**InchiKey:** IJUBFADZGYKUJR-NNJIEVJOSA-N  
**Formula:** C22H30N2O6  
**SMILES:** CCOC(=O)NC(Cc1cn(C(=O)OCC)c2ccccc12)C(=O)OC(C)C(C)C  
**Mol. weight [g/mol]:** 418.48

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	3.891		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
rinpol	2664.80		NIST Webbook
rinpol	2664.80		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=R502215&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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