

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

**InChI:** CCOC(=O)C1=CC=C(C=C1)C(=O)OC(C)C(C)C  
**InChIKey:** CLNFPJLQNJRIWKG-IURRXHLWSA-N  
**Formula:** C<sub>18</sub>H<sub>27</sub>NO<sub>4</sub>  
**SMILES:** CCOC(O)=NC(CCc1ccccc1)C(=O)OC(C)C(C)C  
**Mol. weight [g/mol]:** 321.41

## Physical Properties

Property code	Value	Unit	Source
hf	-650.98	kJ/mol	Joback Method
hvap	88.41	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.526		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2170.90		NIST Webbook
rinpol	2170.90		NIST Webbook
tb	904.05	K	Joback Method
tc	1116.00	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R502097&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcpvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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