

# D-Alanine, N-ethoxycarbonyl-, tetradecyl ester

**Inchi:** InChI=1S/C20H39NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-25-19(22)18(3)21-20(23)2  
**InchiKey:** BHAAAYBCUSJXMR-UHFFFAOYSA-N  
**Formula:** C20H39NO4  
**SMILES:** CCCCCCCCCCCCCOC(=O)C(C)N=C(O)OCC  
**Mol. weight [g/mol]:** 357.53

## Physical Properties

Property code	Value	Unit	Source
hf	-918.23	kJ/mol	Joback Method
hvap	91.36	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.570		Crippen Method
mcvol	317.520	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	924.01	K	Joback Method
tc	1132.03	K	Joback Method

## Sources

**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)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U347757&Units=SI>

## 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>mcvol:</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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