

# Glycine, 2-cyclohexyl-N-(but-3-en-1-yl)oxycarbonyl-, tridecyl ester

InChI: InChI=1S/C26H47NO4/c1-3-5-7-8-9-10-11-12-13-14-18-22-30-25(28)24(23-19-16-15-17-18)/1-2  
InChIKey: JNTBHWBCTZZLIY-UHFFFAOYSA-N

Formula: C<sub>26</sub>H<sub>47</sub>NO<sub>4</sub>

SMILES: C=CCCOC(O)=NC(C=O)OCCCCCCCCCCCCC)C1CCCCC1

Mol. weight [g/mol]: 437.66

## Physical Properties

Property code	Value	Unit	Source
hf	-862.32	kJ/mol	Joback Method
hvap	104.48	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.296		Crippen Method
mcvol	386.900	ml/mol	McGowan Method
pc	846.03	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		NIST Webbook
tb	1077.52	K	Joback Method
tc	1330.11	K	Joback Method

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U383250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383250&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## 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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