

Glycine, 2-cyclohexyl-N-(but-2-yn-1-yl)oxycarbonyl-, undecyl ester

InChI: InChI=1S/C24H41NO4/c1-3-5-7-8-9-10-11-12-16-20-28-23(26)22(21-17-14-13-15-18-21)
InChIKey: ONJGIUPJVIQXEA-UHFFFAOYSA-N

Formula: C24H41NO4

SMILES: CC#CCOC(O)=NC(C=O)OCCCCCCCCCCC1CCCCC1

Mol. weight [g/mol]: 407.59

Physical Properties

Property code	Value	Unit	Source
hf	-674.17	kJ/mol	Joback Method
hvap	102.85	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.963		Crippen Method
mcvol	354.420	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinsol	2887.00		NIST Webbook
rinsol	2887.00		NIST Webbook
tb	1044.08	K	Joback Method
tc	1278.82	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U383222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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

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