Glycine, 2-cyclohexyl-N-(but-3-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)25-24(27)29-19-4-2/h2,21-22H,3,5-20H2,1H3,(H,25,27)

InchiKey: SKCABHVURBQMBX-UHFFFAOYSA-N

Formula: C24H41NO4

SMILES: C#CCCOC(O)=NC(C(=O)OCCCCCCCCCCC)C1CCCCC1

Mol. weight [g/mol]: 407.59

Physical Properties

Property code	Value	Unit	Source
hf	-654.57	kJ/mol	Joback Method
hvap	100.56	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.963		Crippen Method
mcvol	354.420	ml/mol	McGowan Method
pc	1014.24	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	1025.20	K	Joback Method
tc	1256.06	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U383192&Units=SI

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