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

Inchi: InChI=1S/C26H45NO4/c1-3-5-7-8-9-10-11-12-13-14-18-22-30-25(28)24(23-19-16-15-17-

InchiKey: FRFRBYBCDDNNQD-UHFFFAOYSA-N

Formula: C26H45NO4

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

Mol. weight [g/mol]: 435.64

Physical Properties

Property code	Value	Unit	Source
hf	-695.85	kJ/mol	Joback Method
hvap	105.01	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.743		Crippen Method
mcvol	382.600	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	1070.96	K	Joback Method
tc	1317.44	K	Joback Method

Sources

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=U383194&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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