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

Inchi: InChI=1S/C22H37NO4/c1-3-5-7-8-9-10-14-18-26-21(24)20(19-15-12-11-13-16-19)23-22(

InchiKey: JSKRNHJXIGRWIW-UHFFFAOYSA-N

Formula: C22H37NO4

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

Mol. weight [g/mol]: 379.53

Physical Properties

Property code	Value	Unit	Source
hf	-613.29	kJ/mol	Joback Method
hvap	96.10	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.183		Crippen Method
mcvol	326.240	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	2598.00		NIST Webbook
tb	979.44	K	Joback Method
tc	1199.37	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=U383190&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