Glycine, 2-cyclohexyl-N-(but-2-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: DRXGWLHITKPBJU-UHFFFAOYSA-N

Formula: C22H37NO4

SMILES: CC#CCOC(O)=NC(C(=O)OCCCCCCCCC)C1CCCCC1

Mol. weight [g/mol]: 379.53

Physical Properties

Property code	Value	Unit	Source
hf	-632.89	kJ/mol	Joback Method
hvap	98.40	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.183		Crippen Method
mcvol	326.240	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	998.32	K	Joback Method
tc	1222.75	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=U383220&Units=SI

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

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