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

Inchi: InChI=1S/C21H35NO4/c1-3-5-7-8-9-13-17-25-20(23)19(18-14-11-10-12-15-18)22-21(24)
InchiKey: SHXWKHONQQWFSI-UHFFFAOYSA-N
Formula: C21H35NO4
SMILES: CC#CCOC(O)=NC(C(=O)OCCCCCCCC)C1CCCCC1
Mol. weight [g/mol]: 365.51

Physical Properties

Property code	Value	Unit	Source
hf	-612.25	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.793		Crippen Method
mcvol	312.150	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2594.00		NIST Webbook
rinpol	2594.00		NIST Webbook
tb	975.44	K	Joback Method
tc	1196.28	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=U383219&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