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

Inchi: InChI=1S/C19H31NO4/c1-4-5-13-24-19(22)20-17(16-11-7-6-8-12-16)18(21)23-14-9-10-1

InchiKey: QORMMBJJJPIGSR-UHFFFAOYSA-N

Formula: C19H31NO4

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

Mol. weight [g/mol]: 337.45

Physical Properties

Property code	Value	Unit	Source
hf	-556.65	kJ/mol	Joback Method
hvap	89.04	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.869		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2273.00		NIST Webbook
tb	910.36	K	Joback Method
tc	1122.73	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=U383186&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