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

Inchi: InChI=1S/C20H33NO4/c1-3-5-7-8-12-16-24-19(22)18(17-13-10-9-11-14-17)21-20(23)25-

Inchikey: OLHGSYROXMESRL-UHFFFAOYSA-N

Formula: C20H33NO4

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

Mol. weight [g/mol]: 351.48

Physical Properties

Property code	Value	Unit	Source
hf	-572.01	kJ/mol	Joback Method
hvap	91.65	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.403		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	933.68	K	Joback Method
tc	1146.74	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383188&Units=SI

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

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