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

Inchi: InChI=1S/C28H49NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-20-24-32-27(30)26(25-21-18-
InchiKey: YMOCWQRSAJYBOZ-UHFFFAOYSA-N
Formula: C28H49NO4
SMILES: C#CCCOC(O)=NC(C(=O)OCCCCCCCCCCCCCCC)C1CCCCC1
Mol. weight [g/mol]: 463.69

Physical Properties

Property code	Value	Unit	Source
hf	-737.13	kJ/mol	Joback Method
hvap	109.46	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.524		Crippen Method
mcvol	410.780	ml/mol	McGowan Method
pc	805.25	kPa	Joback Method
rinpol	3204.00		NIST Webbook
tb	1116.72	K	Joback Method
tc	1384.19	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383196&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