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

Inchi: InChI=1S/C30H53NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-22-26-34-29(32)28(27-
Inchikey: BNUIUVXZSMXONG-UHFFFAOYSA-N
Formula: C30H53NO4
SMILES: C#CCCOC(O)=NC(C(=O)OCCCCCCCCCCCCCCCCC)C1CCCCC1
Mol. weight [g/mol]: 491.75

Physical Properties

Property code	Value	Unit	Source
hf	-778.41	kJ/mol	Joback Method
hvap	113.91	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.304		Crippen Method
mcvol	438.960	ml/mol	McGowan Method
pc	724.18	kPa	Joback Method
rinpol	3403.00		NIST Webbook
rinpol	3403.00		NIST Webbook
tb	1162.48	K	Joback Method
tc	1457.18	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383198&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