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

Inchi: InChI=1S/C27H47NO4/c1-3-5-7-8-9-10-11-12-13-14-15-19-23-31-26(29)25(24-20-17-16-
InchiKey: WLQMZWRAIRAYRY-UHFFFAOYSA-N
Formula: C27H47NO4
SMILES: C#CCCOC(O)=NC(C(=O)OCCCCCCCCCCCCCC)C1CCCCC1
Mol. weight [g/mol]: 449.67

Physical Properties

Property code	Value	Unit	Source
hf	-716.49	kJ/mol	Joback Method
hvap	107.23	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.134		Crippen Method
mcvol	396.690	ml/mol	McGowan Method
pc	850.98	kPa	Joback Method
rinpol	3104.00		NIST Webbook
rinpol	3104.00		NIST Webbook
tb	1093.84	K	Joback Method
tc	1350.09	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=U383195&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

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