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

Inchi: InChI=1S/C29H51NO4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-21-25-33-28(31)27(26-22-
InchiKey: CJHYKCGUDLGCGC-UHFFFAOYSA-N
Formula: C29H51NO4
SMILES: C#CCCOC(O)=NC(C(=O)OCCCCCCCCCCCCCCCC)C1CCCCC1
Mol. weight [g/mol]: 477.72

Physical Properties

Property code	Value	Unit	Source
hf	-757.77	kJ/mol	Joback Method
hvap	111.69	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	7.914		Crippen Method
mcvol	424.870	ml/mol	McGowan Method
pc	763.10	kPa	Joback Method
rinpol	3304.00		NIST Webbook
rinpol	3304.00		NIST Webbook
tb	1139.60	K	Joback Method
tc	1419.85	K	Joback Method

Sources

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=U383197&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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