

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

InChI: InChI=1S/C19H31NO4/c1-3-5-7-11-15-23-18(21)17(16-12-9-8-10-13-16)20-19(22)24-14
InChIKey: SHWCUIJFTWRLEX-UHFFFAOYSA-N

Formula: C19H31NO4

SMILES: CC#CCOC(O)=NC(C=O)OCCCCC)C1CCCCC1

Mol. weight [g/mol]: 337.45

Physical Properties

Property code	Value	Unit	Source
hf	-570.97	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.013		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	2400.00		NIST Webbook
tb	929.68	K	Joback Method
tc	1146.17	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=U383217&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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