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

InChI:	InChI=1S/C19H31NO4/c1-4-5-13-24-19(22)20-17(16-11-7-6-8-12-16)18(21)23-14-9-10-1
InChiKey:	JVUXGTACJVRTIF-UHFFFAOYSA-N
Formula:	C19H31NO4
SMILES:	CC#CCOC(O)=NC(C(=O)OCCCC(C)C)C1CCCCC1
Mol. weight [g/mol]:	337.45

Physical Properties

Property code	Value	Unit	Source
hf	-576.25	kJ/mol	Joback Method
hvap	91.33	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.869		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
tb	929.24	K	Joback Method
tc	1147.26	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=U383216&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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

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