

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

InChI: InChI=1S/C23H39NO4/c1-3-5-7-8-9-10-11-15-19-27-22(25)21(20-16-13-12-14-17-20)24
InChIKey: QKNSULMWGFYWFD-UHFFFAOYSA-N

Formula: C23H39NO4
SMILES: C#CCCOC(O)=NC(C(=O)OCCCCCCCCCCC)C1CCCCC1
Mol. weight [g/mol]: 393.56

Physical Properties

Property code	Value	Unit	Source
hf	-633.93	kJ/mol	Joback Method
hvap	98.33	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.573		Crippen Method
mcvol	340.330	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	2696.00		NIST Webbook
tb	1002.32	K	Joback Method
tc	1227.17	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383191&Units=SI>

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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