

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

InChI: InChI=1S/C25H43NO4/c1-3-5-7-8-9-10-11-12-13-17-21-29-24(27)23(22-18-15-14-16-19-20)/N1H2C3C4C5C6C7C8C9C10C11C12C13C14C15C16C17C18C19C20C21C22C23C24C25
InChIKey: NHYKKVTWMPVMSG-UHFFFAOYSA-N

Formula: C25H43NO4

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

Mol. weight [g/mol]: 421.61

Physical Properties

Property code	Value	Unit	Source
hf	-694.81	kJ/mol	Joback Method
hvap	105.08	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.353		Crippen Method
mcvol	368.510	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	2986.00		NIST Webbook
rinpol	2986.00		NIST Webbook
tb	1066.96	K	Joback Method
tc	1308.57	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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