

Glycine, 2-cyclohexyl-N-(but-3-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)/1
InChIKey: UGYIPKHBJSWGE-UHFFFAOYSA-N

Formula: C25H43NO4

SMILES: C#CCCOC(O)=NC(C=O)OCCCCCCCCCCCCC1CCCCC1

Mol. weight [g/mol]: 421.61

Physical Properties

Property code	Value	Unit	Source
hf	-675.21	kJ/mol	Joback Method
hvap	102.78	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.353		Crippen Method
mcvol	368.510	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tb	1048.08	K	Joback Method
tc	1286.12	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=U383193&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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