

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

InChI: InChI=1S/C20H33NO4/c1-3-5-7-8-12-16-24-19(22)18(17-13-10-9-11-14-17)21-20(23)25-
InChIKey: BKYZAMKQIFSTDG-UHFFFAOYSA-N

Formula: C20H33NO4

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

Mol. weight [g/mol]: 351.48

Physical Properties

Property code	Value	Unit	Source
hf	-591.61	kJ/mol	Joback Method
hvap	93.95	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.403		Crippen Method
mcvol	298.060	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
tb	952.56	K	Joback Method
tc	1170.78	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383218&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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>

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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