

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

InChI: InChI=1S/C18H29NO4/c1-3-5-10-14-22-17(20)16(15-11-8-7-9-12-15)19-18(21)23-13-6-4
InChIKey: RKUNYJBXDDGATK-UHFFFAOYSA-N

Formula: C18H29NO4
SMILES: C#CCCOC(O)=NC(C(=O)OCCCCC)C1CCCCC1
Mol. weight [g/mol]: 323.43

Physical Properties

Property code	Value	Unit	Source
hf	-530.73	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.623		Crippen Method
mcvol	269.880	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
tb	887.92	K	Joback Method
tc	1097.66	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U383185&Units=SI>
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

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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