

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

InChI: InChI=1S/C19H31NO4/c1-3-5-7-11-15-23-18(21)17(16-12-9-8-10-13-16)20-19(22)24-14
InChIKey: APAHMHXOAWFETC-UHFFFAOYSA-N

Formula: C19H31NO4
SMILES: C#CCCOC(O)=NC(C(=O)OCCCCC)C1CCCCC1
Mol. weight [g/mol]: 337.45

Physical Properties

Property code	Value	Unit	Source
hf	-551.37	kJ/mol	Joback Method
hvap	89.43	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.013		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	2308.00		NIST Webbook
tb	910.80	K	Joback Method
tc	1121.79	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=U383187&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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