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

Inchi: InChI=1S/C17H23NO4/c1-3-5-12-21-16(19)15(14-10-8-7-9-11-14)18-17(20)22-13-6-4-2/h
InchiKey: CVFORSSTDLQCHO-UHFFFAOYSA-N
Formula: C17H23NO4
SMILES: CC#CCOC(=O)NC(C(=O)OCC#CC)C1CCCCC1
Mol. weight [g/mol]: 305.37

Physical Properties

Property code	Value	Unit	Source
gf	141.42	kJ/mol	Joback Method
hf	-236.70	kJ/mol	Joback Method
hfus	45.01	kJ/mol	Joback Method
hvap	82.53	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.251		Crippen Method
mcvol	247.190	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	828.22	K	Joback Method
tc	1061.27	K	Joback Method
tf	682.91	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.94	J/mol×K	828.22	Joback Method
cpg	765.60	J/mol×K	867.06	Joback Method
cpg	780.80	J/mol×K	905.90	Joback Method
cpg	794.56	J/mol×K	944.75	Joback Method
cpg	806.89	J/mol×K	983.59	Joback Method
cpg	817.80	J/mol×K	1022.43	Joback Method
cpg	827.31	J/mol×K	1061.27	Joback Method

Sources

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=U383224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume