Glycine, di(2-cyclohexyl-N-(but-3-en-1-yl)oxycarbonyl)-ester

Inchi: InChI=1S/C17H27NO4/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: IURJMFCQIBCLHG-UHFFFAOYSA-N
Formula: C17H27NO4
SMILES: C=CCCOC(=O)NC(C(=O)OCCC=C)C1CCCCC1
Mol. weight [g/mol]: 309.40

Physical Properties

Property code	Value	Unit	Source
gf	-88.50	kJ/mol	Joback Method
hf	-530.44	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	76.89	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.357		Crippen Method
mcvol	255.790	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2098.00		NIST Webbook
rinpol	2098.00		NIST Webbook
tb	803.58	K	Joback Method
tc	1008.28	K	Joback Method
tf	467.19	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.38	J/mol×K	803.58	Joback Method
cpg	813.19	J/mol×K	837.70	Joback Method
cpg	828.77	J/mol×K	871.81	Joback Method
cpg	843.16	J/mol×K	905.93	Joback Method
cpg	856.39	J/mol×K	940.05	Joback Method
cpg	868.48	J/mol×K	974.16	Joback Method
cpg	879.46	J/mol×K	1008.28	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=U383253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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