Glycine, 2-cyclohexyl-N-isobutoxycarbonyl-, octyl ester

Inchi: InChI=1S/C21H39NO4/c1-4-5-6-7-8-12-15-25-20(23)19(18-13-10-9-11-14-18)22-21(24)2

InchiKey: MTJYGRLLWIUILT-UHFFFAOYSA-N

Formula: C21H39NO4

SMILES: CCCCCCCCOC(=O)C(N=C(O)OCC(C)C)C1CCCCC1

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
hf	-889.83	kJ/mol	Joback Method
hvap	93.63	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.426		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	966.00	K	Joback Method
tc	1182.83	K	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=U383098&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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