Glycine, 2-cyclohexyl-N-(2-ethylhexyl)oxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C21H39NO4/c1-5-7-11-17(6-2)15-26-21(24)22-19(18-12-9-8-10-13-18)20(23)2

InchiKey: PAFLSJGABCJUKN-UHFFFAOYSA-N

Formula: C21H39NO4

SMILES: CCCCC(CC)COC(O)=NC(C(=O)OCC(C)C)C1CCCCC1

Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
hf	-895.11	kJ/mol	Joback Method
hvap	93.24	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.282		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	965.56	K	Joback Method
tc	1182.61	K	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=U383147&Units=SI

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

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