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

Inchi: InChI=1S/C26H49NO4/c1-4-5-6-7-8-9-10-11-12-13-17-20-30-25(28)24(23-18-15-14-16-1

InchiKey: VUZQXWWSNNYLTH-UHFFFAOYSA-N

Formula: C26H49NO4

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

Mol. weight [g/mol]: 439.67

Physical Properties

Property code	Value	Unit	Source
hf	-993.03	kJ/mol	Joback Method
hvap	104.76	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.376		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	2856.00		NIST Webbook
tb	1080.40	K	Joback Method
tc	1334.07	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383103&Units=SI

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

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