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

Inchi: InChI=1S/C25H47NO4/c1-3-5-7-9-11-16-20-29-24(27)23(22-18-14-13-15-19-22)26-25(28

InchiKey: MEPQIYSASSPJKU-UHFFFAOYSA-N

Formula: C25H47NO4

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

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
hf	-967.11	kJ/mol	Joback Method
hvap	102.92	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.130		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
pc	873.25	kPa	Joback Method
rinpol	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	1057.96	K	Joback Method
tc	1303.47	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=U383130&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