Glycine, 2-cyclohexyl-N-propoxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C30H57NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-26-34-29(32)28(2

InchiKey: VDTUWJMIIQLZNR-UHFFFAOYSA-N

Formula: C30H57NO4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(N=C(O)OCCC)C1CCCCC1

Mol. weight [g/mol]: 495.78

Physical Properties

Property code	Value	Unit	Source
hf	-1070.31	kJ/mol	Joback Method
hvap	114.05	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	9.081		Crippen Method
mcvol	447.560	ml/mol	McGowan Method
pc	669.77	kPa	Joback Method
rinpol	3414.00		NIST Webbook
tb	1172.36	K	Joback Method
tc	1485.60	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U383081&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

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

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