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

Inchi: InChI=1S/C29H55NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-21-25-33-28(31)27(26-2

InchiKey: IGQMLOIWDTVZDF-UHFFFAOYSA-N

Formula: C29H55NO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(NC(=O)OCCC)C1CCCCC1

Mol. weight [g/mol]: 481.75

Physical Properties

Property code	Value	Unit	Source
gf	-163.14	kJ/mol	Joback Method
hf	-1028.98	kJ/mol	Joback Method
hfus	69.85	kJ/mol	Joback Method
hvap	104.94	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	8.486		Crippen Method
mcvol	433.470	ml/mol	McGowan Method
pc	736.82	kPa	Joback Method
rinpol	3314.00		NIST Webbook
rinpol	3314.00		NIST Webbook
tb	1084.78	K	Joback Method
tc	1345.76	K	Joback Method
tf	605.95	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1598.94	J/mol×K	1084.78	Joback Method
cpg	1618.59	J/mol×K	1128.28	Joback Method
cpg	1635.73	J/mol×K	1171.77	Joback Method
cpg	1650.48	J/mol×K	1215.27	Joback Method
cpg	1662.94	J/mol×K	1258.77	Joback Method
cpg	1673.22	J/mol×K	1302.26	Joback Method
cpg	1681.45	J/mol×K	1345.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383080&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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume