Glycine, 2-cyclohexyl-N-(3-chloropropoxycarbonyl)-, nonyl ester

Inchi: InChI=1S/C21H38ClNO4/c1-2-3-4-5-6-7-11-16-26-20(24)19(18-13-9-8-10-14-18)23-21(2

InchiKey: IZFUCNGTNDFLPB-UHFFFAOYSA-N

Formula: C21H38ClNO4

SMILES: CCCCCCCCCOC(=O)C(NC(=O)OCCCCl)C1CCCCC1

Mol. weight [g/mol]: 403.98

Physical Properties

Property code	Value	Unit	Source
gf	-242.43	kJ/mol	Joback Method
hf	-879.60	kJ/mol	Joback Method
hfus	53.33	kJ/mol	Joback Method
hvap	91.51	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.584		Crippen Method
mcvol	332.990	ml/mol	McGowan Method
pc	1146.76	kPa	Joback Method
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
tb	939.17	K	Joback Method
tc	1151.28	K	Joback Method
tf	545.71	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.68	J/mol×K	939.17	Joback Method
cpg	1137.42	J/mol×K	974.52	Joback Method
cpg	1152.65	J/mol×K	1009.87	Joback Method
cpg	1166.41	J/mol×K	1045.22	Joback Method
cpg	1178.73	J/mol×K	1080.58	Joback Method
cpg	1189.65	J/mol×K	1115.93	Joback Method
cpg	1199.21	J/mol×K	1151.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392340&Units=SI

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