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

Inchi: InChI=1S/C22H40ClNO4/c1-2-3-4-5-6-7-8-12-17-27-21(25)20(19-14-10-9-11-15-19)24-2

InchiKey: CQAYYOPJBYKRMB-UHFFFAOYSA-N

Formula: C22H40ClNO4

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

Mol. weight [g/mol]: 418.01

Physical Properties

Property code	Value	Unit	Source
gf	-234.01	kJ/mol	Joback Method
hf	-900.24	kJ/mol	Joback Method
hfus	55.92	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.974		Crippen Method
mcvol	347.080	ml/mol	McGowan Method
pc	1075.69	kPa	Joback Method
rinpol	2867.00		NIST Webbook
rinpol	2867.00		NIST Webbook
tb	962.05	K	Joback Method
tc	1178.08	K	Joback Method
tf	556.98	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.43	J/mol×K	962.05	Joback Method
cpg	1199.28	J/mol×K	998.05	Joback Method
cpg	1214.54	J/mol×K	1034.06	Joback Method
cpg	1228.25	J/mol×K	1070.06	Joback Method
cpg	1240.46	J/mol×K	1106.07	Joback Method
cpg	1251.21	J/mol×K	1142.07	Joback Method
cpg	1260.54	J/mol×K	1178.08	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=U392341&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