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

Inchi: InChI=1S/C18H32ClNO4/c1-14(2)8-6-12-23-17(21)16(15-9-4-3-5-10-15)20-18(22)24-13-

InchiKey: JVIYRUWUPFRWJC-UHFFFAOYSA-N

Formula: C18H32ClNO4

SMILES: CC(C)CCCOC(=O)C(NC(=O)OCCCCl)C1CCCCC1

Mol. weight [g/mol]: 361.90

Physical Properties

Property code	Value	Unit	Source
gf	-270.13	kJ/mol	Joback Method
hf	-822.96	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.270		Crippen Method
mcvol	290.720	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	870.09	K	Joback Method
tc	1077.47	K	Joback Method
tf	496.90	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.98	J/mol×K	870.09	Joback Method
cpg	955.56	J/mol×K	904.65	Joback Method
cpg	970.78	J/mol×K	939.22	Joback Method
cpg	984.66	J/mol×K	973.78	Joback Method
cpg	997.23	J/mol×K	1008.34	Joback Method
cpg	1008.51	J/mol×K	1042.90	Joback Method
cpg	1018.52	J/mol×K	1077.47	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=U392344&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