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

Inchi: InChI=1S/C17H30ClNO4/c1-2-3-7-12-22-16(20)15(14-9-5-4-6-10-14)19-17(21)23-13-8-11
InchiKey: IYVMWBQASPGQIN-UHFFFAOYSA-N
Formula: C17H30ClNO4
SMILES: CCCCCOC(=O)C(NC(=O)OCCCCl)C1CCCCC1
Mol. weight [g/mol]: 347.88

Physical Properties

Property code	Value	Unit	Source
gf	-276.11	kJ/mol	Joback Method
hf	-797.04	kJ/mol	Joback Method
hfus	42.97	kJ/mol	Joback Method
hvap	82.61	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.024		Crippen Method
mcvol	276.630	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	847.65	K	Joback Method
tc	1052.77	K	Joback Method
tf	500.63	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.95	J/mol×K	847.65	Joback Method
cpg	895.34	J/mol×K	881.84	Joback Method
cpg	910.44	J/mol×K	916.02	Joback Method
cpg	924.27	J/mol×K	950.21	Joback Method
cpg	936.85	J/mol×K	984.39	Joback Method
cpg	948.21	J/mol×K	1018.58	Joback Method
cpg	958.37	J/mol×K	1052.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392337&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

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