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

Inchi: InChI=1S/C19H34ClNO4/c1-2-3-4-5-9-14-24-18(22)17(16-11-7-6-8-12-16)21-19(23)25-1
Inchikey: SAVVLMDJHQNXPF-UHFFFAOYSA-N
Formula: C19H34ClNO4
SMILES: CCCCCCCOC(=O)C(NC(=O)OCCCCl)C1CCCCC1
Mol. weight [g/mol]: 375.93

Physical Properties

Property code	Value	Unit	Source
gf	-259.27	kJ/mol	Joback Method
hf	-838.32	kJ/mol	Joback Method
hfus	48.15	kJ/mol	Joback Method
hvap	87.06	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.804		Crippen Method
mcvol	304.810	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
rinpol	2576.00		NIST Webbook
rinpol	2576.00		NIST Webbook
tb	893.41	K	Joback Method
tc	1100.40	K	Joback Method
tf	523.17	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.65	J/mol×K	893.41	Joback Method
cpg	1015.21	J/mol×K	927.91	Joback Method
cpg	1030.38	J/mol×K	962.41	Joback Method
cpg	1044.20	J/mol×K	996.91	Joback Method
cpg	1056.69	J/mol×K	1031.41	Joback Method
cpg	1067.88	J/mol×K	1065.91	Joback Method
cpg	1077.80	J/mol×K	1100.40	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=U392338&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