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

Inchi: InChI=1S/C15H25Cl2NO4/c16-8-4-10-21-14(19)13(12-6-2-1-3-7-12)18-15(20)22-11-5-9-17/h12-13H,1-11H2,(H,18,20)

InchiKey: GSZKBSYYYQIVMZ-UHFFFAOYSA-N

Formula: C15H25Cl2NO4

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

Mol. weight [g/mol]: 354.27

Physical Properties

Property code	Value	Unit	Source
gf	-304.88	kJ/mol	Joback Method
hf	-771.50	kJ/mol	Joback Method
hfus	41.98	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.462		Crippen Method
mcvol	260.690	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2481.00		NIST Webbook
tb	839.32	K	Joback Method
tc	1049.41	K	Joback Method
tf	508.01	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.22	J/mol×K	839.32	Joback Method
cpg	804.06	J/mol×K	874.33	Joback Method
cpg	817.66	J/mol×K	909.35	Joback Method
cpg	830.05	J/mol×K	944.36	Joback Method
cpg	841.24	J/mol×K	979.38	Joback Method
cpg	851.25	J/mol×K	1014.39	Joback Method
cpg	860.11	J/mol×K	1049.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392342&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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