Glycine, 2-cyclohexyl-N-(2,2,2-trichloroethoxy)carbonyl-, propyl ester

Inchi: InChI=1S/C14H22Cl3NO4/c1-2-8-21-12(19)11(10-6-4-3-5-7-10)18-13(20)22-9-14(15,16)
InchiKey: BXIZNZWYGUPGTK-UHFFFAOYSA-N
Formula: C14H22Cl3NO4
SMILES: CCCOC(=O)C(NC(=O)OCC(Cl)(Cl)Cl)C1CCCCC1
Mol. weight [g/mol]: 374.69

Physical Properties

Property code	Value	Unit	Source
gf	-322.39	kJ/mol	Joback Method
hf	-775.35	kJ/mol	Joback Method
hfus	36.18	kJ/mol	Joback Method
hvap	83.41	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.985		Crippen Method
mcvol	258.840	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	3374.00		NIST Webbook
rinpol	3374.00		NIST Webbook
tb	850.64	K	Joback Method
tc	1073.32	K	Joback Method
tf	529.08	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.24	J/mol×K	850.64	Joback Method
cpg	771.81	J/mol×K	887.75	Joback Method
cpg	784.13	J/mol×K	924.87	Joback Method
cpg	795.24	J/mol×K	961.98	Joback Method
cpg	805.19	J/mol×K	999.09	Joback Method
cpg	814.03	J/mol×K	1036.21	Joback Method
cpg	821.78	J/mol×K	1073.32	Joback Method

Sources

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=U383116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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