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

Inchi: InChI=1S/C15H24Cl3NO4/c1-10(2)8-22-13(20)12(11-6-4-3-5-7-11)19-14(21)23-9-15(16,
InchiKey: DIJJYKUPSURZAL-UHFFFAOYSA-N
Formula: C15H24Cl3NO4
SMILES: CC(C)COC(=O)C(NC(=O)OCC(Cl)(Cl)Cl)C1CCCCC1
Mol. weight [g/mol]: 388.71

Physical Properties

Property code	Value	Unit	Source
gf	-316.41	kJ/mol	Joback Method
hf	-801.27	kJ/mol	Joback Method
hfus	35.24	kJ/mol	Joback Method
hvap	85.24	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.231		Crippen Method
mcvol	272.930	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	3392.00		NIST Webbook
rinpol	3392.00		NIST Webbook
tb	873.08	K	Joback Method
tc	1096.82	K	Joback Method
tf	525.35	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.80	J/mol×K	873.08	Joback Method
cpg	829.61	J/mol×K	910.37	Joback Method
cpg	842.12	J/mol×K	947.66	Joback Method
cpg	853.36	J/mol×K	984.95	Joback Method
cpg	863.39	J/mol×K	1022.24	Joback Method
cpg	872.26	J/mol×K	1059.53	Joback Method
cpg	880.01	J/mol×K	1096.82	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=U383117&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