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

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

Physical Properties

Property code	Value	Unit	Source
gf	-313.97	kJ/mol	Joback Method
hf	-795.99	kJ/mol	Joback Method
hfus	38.77	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.375		Crippen Method
mcvol	272.930	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	3409.00		NIST Webbook
rinpol	3409.00		NIST Webbook
tb	873.52	K	Joback Method
tc	1094.55	K	Joback Method
tf	540.35	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.25	J/mol×K	873.52	Joback Method
cpg	828.93	J/mol×K	910.36	Joback Method
cpg	841.34	J/mol×K	947.20	Joback Method
cpg	852.53	J/mol×K	984.03	Joback Method
cpg	862.55	J/mol×K	1020.87	Joback Method
cpg	871.44	J/mol×K	1057.71	Joback Method
cpg	879.26	J/mol×K	1094.55	Joback Method

Sources

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=U383118&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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