

# Glycine, 2-cyclohexyl-N-(2,2,2-trichloroethoxy)carbonyl-, 2,2,2-trichloroethyl ester

InChI: ClC1(Cl)C(Cl)C(=O)N(C1CCCC1)C(=O)OCC(Cl)(Cl)Cl  
InChIKey: IFGOIESKTS6BKV-UHFFFAOYSA-N  
Formula: C13H17Cl6NO4  
SMILES: O=C(OCC(Cl)(Cl)Cl)C(N=C(O)OCC(Cl)(Cl)Cl)C1CCCC1  
Mol. weight [g/mol]: 464.00

## Physical Properties

Property code	Value	Unit	Source
hf	-831.37	kJ/mol	Joback Method
hvap	99.93	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.150		Crippen Method
mcpvol	281.470	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	3479.00		NIST Webbook
rinpol	3479.00		NIST Webbook
tb	1001.52	K	Joback Method
tc	1243.51	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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=U383119&Units=SI>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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