# Glycine, 2-cyclohexyl-N-(but-3-en-1-yl)oxycarbonyl-, pentyl ester

**Inchi:** InChI=1S/C18H31NO4/c1-3-5-10-14-22-17(20)16(15-11-8-7-9-12-15)19-18(21)23-13-6-4

**InchiKey:** HYVXPBQSMBFXMV-UHFFFAOYSA-N

**Formula:** C18H31NO4

**SMILES:** C=CCCOC(O)=NC(C(=O)OCCCCC)C1CCCCC1

**Mol. weight [g/mol]:** 325.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -697.20 | kJ/mol | Joback Method |
| hvap | 86.67 | kJ/mol | Joback Method |
| log10ws | -4.40 | | Crippen Method |
| logp | 4.175 | | Crippen Method |
| mcvol | 274.180 | ml/mol | McGowan Method |
| pc | 1402.74 | kPa | Joback Method |
| rinpol | 2195.00 | | NIST Webbook |
| tb | 894.48 | K | Joback Method |
| tc | 1101.57 | 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

**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=U383241&Units=SI

## Legend

**hf:** Enthalpy of formation 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 |