# Carbonic acid, monoamide, N-undecyl-, propyl ester

**Inchi:** InChI=1S/C15H31NO2/c1-3-5-6-7-8-9-10-11-12-13-16-15(17)18-14-4-2/h3-14H2,1-2H3,(

**InchiKey:** WEKPZKWKXWNAFE-UHFFFAOYSA-N

**Formula:** C15H31NO2

**SMILES:** CCCCCCCCCCCN=C(O)OCCC

**Mol. weight [g/mol]:** 257.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -564.95 | kJ/mol | Joback Method |
| hvap | 71.47 | kJ/mol | Joback Method |
| log10ws | -4.67 | | Crippen Method |
| logp | 4.858 | | Crippen Method |
| mcvol | 239.630 | ml/mol | McGowan Method |
| pc | 1389.18 | kPa | Joback Method |
| rinpol | 2233.00 | | NIST Webbook |
| rinpol | 2233.00 | | NIST Webbook |
| tb | 733.76 | K | Joback Method |
| tc | 909.33 | K | Joback Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U415256&Units=SI

**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

## 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 |