# Carbonic acid, but-2-yn-1-yl nonyl ester

**Inchi:** InChI=1S/C14H24O3/c1-3-5-7-8-9-10-11-13-17-14(15)16-12-6-4-2/h3,5,7-13H2,1-2H3
**InchiKey:** BINCOBLXQNPJDN-UHFFFAOYSA-N
**Formula:** C14H24O3
**SMILES:** CC#CCOC(=O)OCCCCCCCCC
**Mol. weight [g/mol]:** 240.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -69.12 | kJ/mol | Joback Method |
| hf | -437.01 | kJ/mol | Joback Method |
| hfus | 39.11 | kJ/mol | Joback Method |
| hvap | 60.48 | kJ/mol | Joback Method |
| log10ws | -4.41 | | Crippen Method |
| logp | 3.913 | | Crippen Method |
| mcvol | 212.830 | ml/mol | McGowan Method |
| pc | 1775.84 | kPa | Joback Method |
| rinpol | 1734.00 | | NIST Webbook |
| rinpol | 1734.00 | | NIST Webbook |
| tb | 627.43 | K | Joback Method |
| tc | 811.37 | K | Joback Method |
| tf | 448.03 | K | Joback Method |
| vc | 0.824 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 556.57 | J/mol×K | 627.43 | Joback Method |
| cpg | 572.78 | J/mol×K | 658.09 | Joback Method |
| cpg | 588.28 | J/mol×K | 688.74 | Joback Method |
| cpg | 603.08 | J/mol×K | 719.40 | Joback Method |
| cpg | 617.19 | J/mol×K | 750.06 | Joback Method |
| cpg | 630.60 | J/mol×K | 780.72 | Joback Method |
| cpg | 643.31 | J/mol×K | 811.37 | Joback Method |

# Sources

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|---|---|
| **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=U383205&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **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 |