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

**Inchi:** InChI=1S/C20H36O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-23-20(21)22-18-6-4-2/h3
**InchiKey:** WBJRILGOHMFYFZ-UHFFFAOYSA-N
**Formula:** C20H36O3
**SMILES:** CC#CCOC(=O)OCCCCCCCCCCCCCCC
**Mol. weight [g/mol]:** 324.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -18.60 | kJ/mol | Joback Method |
| hf | -560.85 | kJ/mol | Joback Method |
| hfus | 54.65 | kJ/mol | Joback Method |
| hvap | 73.83 | kJ/mol | Joback Method |
| log10ws | -6.92 | | Crippen Method |
| logp | 6.254 | | Crippen Method |
| mcvol | 297.370 | ml/mol | McGowan Method |
| pc | 1149.87 | kPa | Joback Method |
| rinpol | 2328.00 | | NIST Webbook |
| rinpol | 2328.00 | | NIST Webbook |
| tb | 764.71 | K | Joback Method |
| tc | 946.72 | K | Joback Method |
| tf | 515.65 | K | Joback Method |
| vc | 1.159 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 895.17 | J/mol×K | 764.71 | Joback Method |
| cpg | 913.91 | J/mol×K | 795.05 | Joback Method |
| cpg | 931.69 | J/mol×K | 825.38 | Joback Method |
| cpg | 948.53 | J/mol×K | 855.72 | Joback Method |
| cpg | 964.42 | J/mol×K | 886.05 | Joback Method |
| cpg | 979.40 | J/mol×K | 916.39 | Joback Method |
| cpg | 993.48 | J/mol×K | 946.72 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U383210&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 |

# 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 |