

# Carbonic acid, but-3-yn-1-yl heptyl ester

|                      |                                                                         |
|----------------------|-------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H20O3/c1-3-5-7-8-9-11-15-12(13)14-10-6-4-2/h2H,3,5-11H2,1H3 |
| InchiKey:            | HRLOVJPHCNEVAK-UHFFFAOYSA-N                                             |
| Formula:             | C12H20O3                                                                |
| SMILES:              | C#CCCOC(=O)OCCCCCCC                                                     |
| Mol. weight [g/mol]: | 212.29                                                                  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -65.69  | kJ/mol  | Joback Method  |
| hf            | -376.13 | kJ/mol  | Joback Method  |
| hfus          | 33.79   | kJ/mol  | Joback Method  |
| hvap          | 53.73   | kJ/mol  | Joback Method  |
| log10ws       | -3.57   |         | Crippen Method |
| logp          | 3.133   |         | Crippen Method |
| mcvol         | 184.650 | ml/mol  | McGowan Method |
| pc            | 2079.33 | kPa     | Joback Method  |
| tb            | 562.79  | K       | Joback Method  |
| tc            | 741.71  | K       | Joback Method  |
| tf            | 366.36  | K       | Joback Method  |
| vc            | 0.712   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 452.00 | J/mol×K | 562.79          | Joback Method |
| cpg           | 466.40 | J/mol×K | 592.61          | Joback Method |
| cpg           | 480.22 | J/mol×K | 622.43          | Joback Method |
| cpg           | 493.46 | J/mol×K | 652.25          | Joback Method |
| cpg           | 506.12 | J/mol×K | 682.07          | Joback Method |
| cpg           | 518.22 | J/mol×K | 711.89          | Joback Method |
| cpg           | 529.75 | J/mol×K | 741.71          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U383174&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383174&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | 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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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