

# Octanoic acid, but-3-yn-2-yl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C12H20O2/c1-4-6-7-8-9-10-12(13)14-11(3)5-2/h2,11H,4,6-10H2,1,3H3 |
| <b>InchiKey:</b>            | JGTVWNZUWKACIY-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H20O2  |
| <b>SMILES:</b>              | C#CC(C)OC(=O)CCCCCCC  |
| <b>Mol. weight [g/mol]:</b> | 196.29  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 36.87   | kJ/mol               | Joback Method  |
| hf            | -249.19 | kJ/mol               | Joback Method  |
| hfus          | 29.07   | kJ/mol               | Joback Method  |
| hvap          | 50.93   | kJ/mol               | Joback Method  |
| log10ws       | -3.61   |                      | Crippen Method |
| logp          | 2.912   |                      | Crippen Method |
| mcvol         | 178.780 | ml/mol               | McGowan Method |
| pc            | 2127.56 | kPa                  | Joback Method  |
| rinqol        | 1306.00 |                      | NIST Webbook   |
| tb            | 539.93  | K                    | Joback Method  |
| tc            | 723.20  | K                    | Joback Method  |
| tf            | 329.13  | K                    | Joback Method  |
| vc            | 0.688   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 425.95 | J/mol×K | 539.93          | Joback Method |
| cpg           | 440.93 | J/mol×K | 570.48          | Joback Method |
| cpg           | 455.25 | J/mol×K | 601.02          | Joback Method |
| cpg           | 468.94 | J/mol×K | 631.57          | Joback Method |
| cpg           | 481.99 | J/mol×K | 662.11          | Joback Method |
| cpg           | 494.43 | J/mol×K | 692.66          | Joback Method |
| cpg           | 506.27 | J/mol×K | 723.20          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U299340&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299340&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvac:</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>mccol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <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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