

# But-3-enyl ethyl carbonate

Inchi:

InChI=1S/C7H12O3/c1-3-5-6-10-7(8)9-4-2/h3H,1,4-6H2,2H3

InchiKey:

ITTRDLLFMNAORT-UHFFFAOYSA-N

Formula:

C7H12O3

SMILES:

C=CCCOC(=O)OCC

Mol. weight [g/mol]:

144.17

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -243.02 | kJ/mol  | Joback Method  |
| hf            | -439.40 | kJ/mol  | Joback Method  |
| hfus          | 16.58   | kJ/mol  | Joback Method  |
| hvap          | 42.07   | kJ/mol  | Joback Method  |
| log10ws       | -1.53   |         | Crippen Method |
| logp          | 1.736   |         | Crippen Method |
| mcvol         | 118.500 | ml/mol  | McGowan Method |
| pc            | 3022.28 | kPa     | Joback Method  |
| rinpol        | 962.00  |         | NIST Webbook   |
| tb            | 454.95  | K       | Joback Method  |
| tc            | 634.51  | K       | Joback Method  |
| tf            | 261.28  | K       | Joback Method  |
| vc            | 0.451   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 245.27    | J/mol×K | 454.95          | Joback Method |
| cpg           | 255.58    | J/mol×K | 484.88          | Joback Method |
| cpg           | 265.55    | J/mol×K | 514.80          | Joback Method |
| cpg           | 275.20    | J/mol×K | 544.73          | Joback Method |
| cpg           | 284.52    | J/mol×K | 574.65          | Joback Method |
| cpg           | 293.49    | J/mol×K | 604.58          | Joback Method |
| cpg           | 302.12    | J/mol×K | 634.51          | Joback Method |
| dvisc         | 0.0022166 | Pa×s    | 261.28          | Joback Method |
| dvisc         | 0.0012324 | Pa×s    | 293.56          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0007698 | Pa×s | 325.84 | Joback Method |
| dvisc | 0.0005234 | Pa×s | 358.12 | Joback Method |
| dvisc | 0.0003793 | Pa×s | 390.39 | Joback Method |
| dvisc | 0.0002887 | Pa×s | 422.67 | Joback Method |
| dvisc | 0.0002284 | Pa×s | 454.95 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U373773&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373773&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>                                 |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>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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