

# 3-Butenyl chloroformate

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C5H7ClO2/c1-2-3-4-8-5(6)7/h2H,1,3-4H2 |
| <b>InchiKey:</b>            | KLDLHTWQLPMOGM-UHFFFAOYSA-N                    |
| <b>Formula:</b>             | C5H7ClO2                                       |
| <b>SMILES:</b>              | C=CCCOC(=O)Cl                                  |
| <b>Mol. weight [g/mol]:</b> | 134.56   |
| <b>CAS:</b>                 | 88986-45-2                                     |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -166.79 | kJ/mol               | Joback Method  |
| hf            | -281.64 | kJ/mol               | Joback Method  |
| hfus          | 14.41   | kJ/mol               | Joback Method  |
| hvap          | 39.59   | kJ/mol               | Joback Method  |
| log10ws       | -1.76   |                      | Crippen Method |
| logp          | 1.938   |                      | Crippen Method |
| mvol          | 96.690  | ml/mol               | McGowan Method |
| pc            | 3686.49 | kPa                  | Joback Method  |
| rinpol        | 832.00  |                      | NIST Webbook   |
| rinpol        | 832.00  |                      | NIST Webbook   |
| tb            | 424.20  | K                    | Joback Method  |
| tc            | 614.21  | K                    | Joback Method  |
| tf            | 246.43  | K                    | Joback Method  |
| vc            | 0.369   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 171.64 | J/mol×K | 424.20          | Joback Method |
| cpg           | 206.45 | J/mol×K | 582.54          | Joback Method |
| cpg           | 200.06 | J/mol×K | 550.88          | Joback Method |
| cpg           | 193.40 | J/mol×K | 519.21          | Joback Method |
| cpg           | 186.44 | J/mol×K | 487.54          | Joback Method |
| cpg           | 179.18 | J/mol×K | 455.87          | Joback Method |
| cpg           | 212.54 | J/mol×K | 614.21          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003131 | Paxs | 424.20 | Joback Method |
| dvisc | 0.0003911 | Paxs | 394.57 | Joback Method |
| dvisc | 0.0005064 | Paxs | 364.94 | Joback Method |
| dvisc | 0.0006863 | Paxs | 335.32 | Joback Method |
| dvisc | 0.0009866 | Paxs | 305.69 | Joback Method |
| dvisc | 0.0015332 | Paxs | 276.06 | Joback Method |
| dvisc | 0.0026492 | Paxs | 246.43 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                             |
| <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=C88986452&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88986452&amp;Units=SI</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>mvol:</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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