

# Butanoic acid, 4-chloro, 1-methylethyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C7H13ClO2/c1-6(2)10-7(9)4-3-5-8/h6H,3-5H2,1-2H3 |
| InchiKey:            | JNUHPPXYHXKRFA-UHFFFAOYSA-N                              |
| Formula:             | C7H13ClO2  |
| SMILES:              | CC(C)OC(=O)CCCCl   |
| Mol. weight [g/mol]: | 164.63   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -240.23 | kJ/mol  | Joback Method  |
| hf            | -453.63 | kJ/mol  | Joback Method  |
| hfus          | 17.35   | kJ/mol  | Joback Method  |
| hvap          | 44.33   | kJ/mol  | Joback Method  |
| log10ws       | -1.88   |         | Crippen Method |
| logp          | 1.957   |         | Crippen Method |
| mcvol         | 129.170 | ml/mol  | McGowan Method |
| pc            | 2850.52 | kPa     | Joback Method  |
| rinpol        | 1048.00 |         | NIST Webbook   |
| rinpol        | 1055.00 |         | NIST Webbook   |
| rinpol        | 1053.00 |         | NIST Webbook   |
| rinpol        | 1039.00 |         | NIST Webbook   |
| rinpol        | 1033.00 |         | NIST Webbook   |
| ripol         | 1466.00 |         | NIST Webbook   |
| ripol         | 1466.00 |         | NIST Webbook   |
| ripol         | 1456.00 |         | NIST Webbook   |
| ripol         | 1459.00 |         | NIST Webbook   |
| ripol         | 1482.00 |         | NIST Webbook   |
| tb            | 472.84  | K       | Joback Method  |
| tc            | 659.46  | K       | Joback Method  |
| tf            | 255.73  | K       | Joback Method  |
| vc            | 0.494   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-------|------|-----------------|--------|
|---------------|-------|------|-----------------|--------|

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 265.41    | J/molxK | 472.84 | Joback Method |
| cpg   | 276.52    | J/molxK | 503.94 | Joback Method |
| cpg   | 287.19    | J/molxK | 535.05 | Joback Method |
| cpg   | 297.44    | J/molxK | 566.15 | Joback Method |
| cpg   | 307.25    | J/molxK | 597.25 | Joback Method |
| cpg   | 316.63    | J/molxK | 628.35 | Joback Method |
| cpg   | 325.59    | J/molxK | 659.46 | Joback Method |
| dvisc | 0.0043091 | Paxs    | 255.73 | Joback Method |
| dvisc | 0.0020358 | Paxs    | 291.92 | Joback Method |
| dvisc | 0.0011348 | Paxs    | 328.10 | Joback Method |
| dvisc | 0.0007104 | Paxs    | 364.28 | Joback Method |
| dvisc | 0.0004840 | Paxs    | 400.47 | Joback Method |
| dvisc | 0.0003514 | Paxs    | 436.65 | Joback Method |
| dvisc | 0.0002680 | Paxs    | 472.84 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R28906&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R28906&amp;Units=SI</a> |
| <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>                   |

## 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>mccvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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