# Butanoic acid, 1,1-dimethylethyl ester

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|---|---|
| **Other names:** | CH3CH2CH2C(O)OC(CH3)3 |
| | tert-Butyl butyrate |
| **Inchi:** | InChI=1S/C8H16O2/c1-5-6-7(9)10-8(2,3)4/h5-6H2,1-4H3 |
| **InchiKey:** | TWBUVVYSQBFVGZ-UHFFFAOYSA-N |
| **Formula:** | C8H16O2 |
| **SMILES:** | CCCC(=O)OC(C)(C)C |
| **Mol. weight [g/mol]:** | 144.21 |
| **CAS:** | 2308-38-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -214.60 | kJ/mol | Joback Method |
| hf | -462.00 | kJ/mol | Joback Method |
| hfus | 11.85 | kJ/mol | Joback Method |
| hvap | 41.26 | kJ/mol | Joback Method |
| log10ws | -2.15 | | Crippen Method |
| logp | 2.128 | | Crippen Method |
| mcvol | 131.020 | ml/mol | McGowan Method |
| pc | 2709.85 | kPa | Joback Method |
| rinpol | 862.00 | | NIST Webbook |
| rinpol | 866.00 | | NIST Webbook |
| rinpol | 873.00 | | NIST Webbook |
| rinpol | 873.00 | | NIST Webbook |
| rinpol | 851.00 | | NIST Webbook |
| rinpol | 858.00 | | NIST Webbook |
| ripol | 1058.00 | | NIST Webbook |
| ripol | 1048.00 | | NIST Webbook |
| ripol | 1037.00 | | NIST Webbook |
| ripol | 1060.00 | | NIST Webbook |
| ripol | 1090.00 | | NIST Webbook |
| tb | 409.40 ± 2.00 | K | NIST Webbook |
| tc | 641.54 | K | Joback Method |
| tf | 254.50 | K | Joback Method |
| vc | 0.496 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 282.32 | J/mol×K | 455.50 | Joback Method |
| cpg | 295.73 | J/mol×K | 486.51 | Joback Method |
| cpg | 308.53 | J/mol×K | 517.51 | Joback Method |
| cpg | 320.73 | J/mol×K | 548.52 | Joback Method |
| cpg | 332.35 | J/mol×K | 579.53 | Joback Method |
| cpg | 343.41 | J/mol×K | 610.54 | Joback Method |
| cpg | 353.92 | J/mol×K | 641.54 | Joback Method |
| dvisc | 0.0046923 | Pa×s | 254.50 | Joback Method |
| dvisc | 0.0021847 | Pa×s | 288.00 | Joback Method |
| dvisc | 0.0011929 | Pa×s | 321.50 | Joback Method |
| dvisc | 0.0007301 | Pa×s | 355.00 | Joback Method |
| dvisc | 0.0004864 | Pa×s | 388.50 | Joback Method |
| dvisc | 0.0003456 | Pa×s | 422.00 | Joback Method |
| dvisc | 0.0002582 | Pa×s | 455.50 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2308385&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |

| | |
|---|---|
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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