# Butanoic acid, 2-oxo-, methyl ester

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| **Other names:** | Butyric acid, 2-oxo-, methyl ester |
| | Methyl «alpha»-oxobutyrate |
| | Methyl 2-oxobutyrate |
| | Methyl ester of 2-oxobutanoic acid |
| | 2-Ketobutyric acid, methyl ester |
| | Methyl 2-oxobutanoate |
| **Inchi:** | InChI=1S/C5H8O3/c1-3-4(6)5(7)8-2/h3H2,1-2H3 |
| **InchiKey:** | XPIWVCAMONZQCP-UHFFFAOYSA-N |
| **Formula:** | C5H8O3 |
| **SMILES:** | CCC(=O)C(=O)OC |
| **Mol. weight [g/mol]:** | 116.12 |
| **CAS:** | 3952-66-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -371.62 | kJ/mol | Joback Method |
| hf | -503.91 | kJ/mol | Joback Method |
| hfus | 13.09 | kJ/mol | Joback Method |
| hvap | 42.63 | kJ/mol | Joback Method |
| log10ws | -0.06 | | Crippen Method |
| logp | 0.138 | | Crippen Method |
| mcvol | 90.320 | ml/mol | McGowan Method |
| pc | 3960.52 | kPa | Joback Method |
| rinpol | 832.40 | | NIST Webbook |
| ripol | 1372.00 | | NIST Webbook |
| ripol | 1375.00 | | NIST Webbook |
| tb | 443.96 | K | Joback Method |
| tc | 634.74 | K | Joback Method |
| tf | 268.20 | K | Joback Method |
| vc | 0.345 | m3/kmol | Joback Method |

## Temperature Dependent Properties

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

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|---|---|---|---|---|
| cpg | 176.41 | J/mol×K | 443.96 | Joback Method |
| cpg | 184.43 | J/mol×K | 475.76 | Joback Method |
| cpg | 192.17 | J/mol×K | 507.55 | Joback Method |
| cpg | 199.65 | J/mol×K | 539.35 | Joback Method |
| cpg | 206.83 | J/mol×K | 571.15 | Joback Method |
| cpg | 213.74 | J/mol×K | 602.95 | Joback Method |
| cpg | 220.34 | J/mol×K | 634.74 | Joback Method |
| dvisc | 0.0025634 | Pa×s | 268.20 | Joback Method |
| dvisc | 0.0015356 | Pa×s | 297.49 | Joback Method |
| dvisc | 0.0010084 | Pa×s | 326.79 | Joback Method |
| dvisc | 0.0007096 | Pa×s | 356.08 | Joback Method |
| dvisc | 0.0005268 | Pa×s | 385.37 | Joback Method |
| dvisc | 0.0004079 | Pa×s | 414.67 | Joback Method |
| dvisc | 0.0003266 | Pa×s | 443.96 | Joback Method |

# Sources

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|---|---|
| **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=C3952667&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |

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

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