# Butanoic acid, 2-hydroxy-3-methyl-

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|---|---|
| **Other names:** | 2-hydroxy-3-methylbutyric acid |
| | 2-Hydroxy-3-methylbutanoic acid |
| **Inchi:** | InChI=1S/C5H10O3/c1-3(2)4(6)5(7)8/h3-4,6H,1-2H3,(H,7,8) |
| **InchiKey:** | NGEWQZIDQIYUNV-UHFFFAOYSA-N |
| **Formula:** | C5H10O3 |
| **SMILES:** | CC(C)C(O)C(=O)O |
| **Mol. weight [g/mol]:** | 118.13 |
| **CAS:** | 4026-18-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -416.22 | kJ/mol | Joback Method |
| hf | -574.13 | kJ/mol | Joback Method |
| hfus | 11.44 | kJ/mol | Joback Method |
| hvap | 66.05 | kJ/mol | Joback Method |
| log10ws | -0.15 | | Crippen Method |
| logp | 0.088 | | Crippen Method |
| mcvol | 94.620 | ml/mol | McGowan Method |
| pc | 4856.20 | kPa | Joback Method |
| rinpol | 1063.30 | | NIST Webbook |
| rinpol | 1063.30 | | NIST Webbook |
| tb | 551.15 | K | Joback Method |
| tc | 723.83 | K | Joback Method |
| tf | 287.68 | K | Joback Method |
| vc | 0.347 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 224.94 | J/mol×K | 551.15 | Joback Method |
| cpg | 232.15 | J/mol×K | 579.93 | Joback Method |
| cpg | 239.04 | J/mol×K | 608.71 | Joback Method |
| cpg | 245.61 | J/mol×K | 637.49 | Joback Method |
| cpg | 251.87 | J/mol×K | 666.27 | Joback Method |

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|---|---|---|---|---|
| cpg | 257.83 | J/mol×K | 695.05 | Joback Method |
| cpg | 263.50 | J/mol×K | 723.83 | Joback Method |
| dvisc | 0.1142973 | Pa×s | 287.68 | Joback Method |
| dvisc | 0.0141241 | Pa×s | 331.59 | Joback Method |
| dvisc | 0.0028462 | Pa×s | 375.50 | Joback Method |
| dvisc | 0.0008021 | Pa×s | 419.41 | Joback Method |
| dvisc | 0.0002874 | Pa×s | 463.33 | Joback Method |
| dvisc | 0.0001230 | Pa×s | 507.24 | Joback Method |
| dvisc | 0.0000603 | Pa×s | 551.15 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C4026180&Units=SI
**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

# 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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume