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

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|---|---|
| **Other names:** | Butyric acid, 3-hydroxy-3-methyl-<br>«beta»-Hydroxy-isovaleric acid<br>3-Hydroxyisovaleric acid<br>3-Hydroxy-3-methylbutanoic acid |
| **Inchi:** | InChI=1S/C5H10O3/c1-5(2,8)3-4(6)7/h8H,3H2,1-2H3,(H,6,7) |
| **InchiKey:** | AXFYFNCPONWUHW-UHFFFAOYSA-N |
| **Formula:** | C5H10O3 |
| **SMILES:** | CC(C)(O)CC(=O)O |
| **Mol. weight [g/mol]:** | 118.13 |
| **CAS:** | 625-08-1 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -408.50 | kJ/mol | Joback Method |
| hf | -572.32 | kJ/mol | Joback Method |
| hfus | 11.07 | kJ/mol | Joback Method |
| hvap | 65.53 | kJ/mol | Joback Method |
| log10ws | -0.39 | | Crippen Method |
| logp | 0.232 | | Crippen Method |
| mcvol | 94.620 | ml/mol | McGowan Method |
| pc | 4876.56 | kPa | Joback Method |
| rinpol | 985.20 | | NIST Webbook |
| rinpol | 985.20 | | NIST Webbook |
| tb | 548.80 | K | Joback Method |
| tc | 724.01 | K | Joback Method |
| tf | 320.10 | K | Joback Method |
| vc | 0.348 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 228.03 | J/mol×K | 548.80 | Joback Method |
| cpg | 235.28 | J/mol×K | 578.00 | Joback Method |
| cpg | 242.14 | J/mol×K | 607.20 | Joback Method |

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|---|---|---|---|---|
| cpg | 248.61 | J/mol×K | 636.41 | Joback Method |
| cpg | 254.72 | J/mol×K | 665.61 | Joback Method |
| cpg | 260.49 | J/mol×K | 694.81 | Joback Method |
| cpg | 265.93 | J/mol×K | 724.01 | Joback Method |
| dvisc | 0.0296306 | Pa×s | 320.10 | Joback Method |
| dvisc | 0.0061970 | Pa×s | 358.22 | Joback Method |
| dvisc | 0.0017512 | Pa×s | 396.33 | Joback Method |
| dvisc | 0.0006177 | Pa×s | 434.45 | Joback Method |
| dvisc | 0.0002578 | Pa×s | 472.57 | Joback Method |
| dvisc | 0.0001226 | Pa×s | 510.68 | Joback Method |
| dvisc | 0.0000646 | Pa×s | 548.80 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C625081&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