# Butanoic acid, 3-hydroxy-, methyl ester, (S)-

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|---|---|
| **Other names:** | Methyl (S)-(+)-3-hydroxybutyrate<br>Butanoic acid, 3-hydroxy-, methyl ester, (3S)-<br>(+)-(3S)-3-Hydroxybutanoic acid methyl ester<br>(S)-3-Hydroxybutanoic acid methyl ester<br>(S)-Methyl 3-hydroxybutanoate<br>(.+/-.)-3-Hydroxybutyric acid, methyl ester<br>methyl (S)-3-hydroxybutyrate |
| **Inchi:** | InChI=1S/C5H10O3/c1-4(6)3-5(7)8-2/h4,6H,3H2,1-2H3/t4-/m1/s1 |
| **InchiKey:** | LDLDJEAVRNAEBW-SCSAIBSYSA-N |
| **Formula:** | C5H10O3 |
| **SMILES:** | COC(=O)CC(C)O |
| **Mol. weight [g/mol]:** | 118.13 |
| **CAS:** | 53562-86-0 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -381.96 | kJ/mol | Joback Method |
| hf | -548.84 | kJ/mol | Joback Method |
| hfus | 12.06 | kJ/mol | Joback Method |
| hvap | 52.17 | kJ/mol | Joback Method |
| log10ws | -0.15 | | Crippen Method |
| logp | -0.070 | | Crippen Method |
| mcvol | 94.620 | ml/mol | McGowan Method |
| pc | 4151.61 | kPa | Joback Method |
| tb | 481.83 | K | Joback Method |
| tc | 657.66 | K | Joback Method |
| tf | 264.09 | K | Joback Method |
| vc | 0.352 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 204.80 | J/mol×K | 481.83 | Joback Method |
| cpg | 241.86 | J/mol×K | 628.35 | Joback Method |

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|---|---|---|---|---|
| cpg | 235.00 | J/mol×K | 599.05 | Joback Method |
| cpg | 227.87 | J/mol×K | 569.74 | Joback Method |
| cpg | 220.46 | J/mol×K | 540.44 | Joback Method |
| cpg | 212.77 | J/mol×K | 511.13 | Joback Method |
| cpg | 248.43 | J/mol×K | 657.66 | Joback Method |
| dvisc | 0.0001769 | Pa×s | 481.83 | Joback Method |
| dvisc | 0.0002891 | Pa×s | 445.54 | Joback Method |
| dvisc | 0.0005156 | Pa×s | 409.25 | Joback Method |
| dvisc | 0.0010292 | Pa×s | 372.96 | Joback Method |
| dvisc | 0.0023843 | Pa×s | 336.67 | Joback Method |
| dvisc | 0.0067671 | Pa×s | 300.38 | Joback Method |
| dvisc | 0.0255824 | Pa×s | 264.09 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 336.20 | K | 1.30 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C53562860&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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