# 1-Butanol, 2-methyl-, propanoate

**Other names:** 1-Butanol, 2-methyl-, propionate
2-Methylbutyl propanoate
2-Methylbutyl propionate
**Inchi:** InChI=1S/C8H16O2/c1-4-7(3)6-10-8(9)5-2/h7H,4-6H2,1-3H3
**InchiKey:** MVJLYXCJBPXRCY-UHFFFAOYSA-N
**Formula:** C8H16O2
**SMILES:** CCC(=O)OCC(C)CC
**Mol. weight [g/mol]:** 144.21
**CAS:** 2438-20-2

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -219.88 | kJ/mol | Joback Method |
| hf | -458.53 | kJ/mol | Joback Method |
| hfus | 15.74 | kJ/mol | Joback Method |
| hvap | 42.17 | kJ/mol | Joback Method |
| log10ws | -1.79 | | Crippen Method |
| logp | 1.986 | | Crippen Method |
| mcvol | 131.020 | ml/mol | McGowan Method |
| pc | 2679.08 | kPa | Joback Method |
| rinpol | 961.00 | | NIST Webbook |
| rinpol | 961.00 | | NIST Webbook |
| rinpol | 962.00 | | NIST Webbook |
| rinpol | 955.00 | | NIST Webbook |
| rinpol | 954.00 | | NIST Webbook |
| rinpol | 975.60 | | NIST Webbook |
| rinpol | 955.00 | | NIST Webbook |
| rinpol | 968.40 | | NIST Webbook |
| rinpol | 950.00 | | NIST Webbook |
| ripol | 1194.00 | | NIST Webbook |
| ripol | 1192.00 | | NIST Webbook |
| ripol | 1189.00 | | NIST Webbook |
| ripol | 1173.00 | | NIST Webbook |
| ripol | 1197.00 | | NIST Webbook |
| ripol | 1197.00 | | NIST Webbook |
| ripol | 1180.00 | | NIST Webbook |
| ripol | 1199.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1199.00 | | NIST Webbook |
| ripol | 1199.00 | | NIST Webbook |
| ripol | 1199.00 | | NIST Webbook |
| tb | 458.29 | K | Joback Method |
| tc | 637.16 | K | Joback Method |
| tf | 237.08 | K | Joback Method |
| vc | 0.501 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 279.83 | J/mol×K | 458.29 | Joback Method |
| cpg | 292.41 | J/mol×K | 488.10 | Joback Method |
| cpg | 304.54 | J/mol×K | 517.91 | Joback Method |
| cpg | 316.22 | J/mol×K | 547.72 | Joback Method |
| cpg | 327.44 | J/mol×K | 577.53 | Joback Method |
| cpg | 338.23 | J/mol×K | 607.34 | Joback Method |
| cpg | 348.57 | J/mol×K | 637.16 | Joback Method |
| dvisc | 0.0048246 | Pa×s | 237.08 | Joback Method |
| dvisc | 0.0020946 | Pa×s | 273.95 | Joback Method |
| dvisc | 0.0011084 | Pa×s | 310.82 | Joback Method |
| dvisc | 0.0006713 | Pa×s | 347.69 | Joback Method |
| dvisc | 0.0004476 | Pa×s | 384.55 | Joback Method |
| dvisc | 0.0003204 | Pa×s | 421.42 | Joback Method |
| dvisc | 0.0002420 | Pa×s | 458.29 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.38601e+01 |
| Coeff. B | -3.48925e+03 |
| Coeff. C | -5.84380e+01 |
| Temperature range (K), min. | 315.52 |
| Temperature range (K), max. | 466.60 |

# Sources

| | |
|---|---|
| **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=C2438202&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **pvap:** | Vapor 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 |