# Pentanoic acid, 2-hydroxy-4-methyl-, ethyl ester

**Other names:** Ethyl 2-hydroxy-4-methylpentanoate
ethyl 2-hydroxy-4-methylvalerate
**Inchi:** InChI=1S/C8H16O3/c1-4-11-8(10)7(9)5-6(2)3/h6-7,9H,4-5H2,1-3H3
**InchiKey:** QRHOWVDPHIXNEN-UHFFFAOYSA-N
**Formula:** C8H16O3
**SMILES:** CCOC(=O)C(O)CC(C)C
**Mol. weight [g/mol]:** 160.21
**CAS:** 10348-47-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -359.14 | kJ/mol | Joback Method |
| hf | -616.04 | kJ/mol | Joback Method |
| hfus | 16.30 | kJ/mol | Joback Method |
| hvap | 58.46 | kJ/mol | Joback Method |
| log10ws | -1.17 | | Crippen Method |
| logp | 0.956 | | Crippen Method |
| mcvol | 136.890 | ml/mol | McGowan Method |
| pc | 2979.54 | kPa | Joback Method |
| rinpol | 1060.00 | | NIST Webbook |
| rinpol | 1078.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |
| rinpol | 1078.00 | | NIST Webbook |
| rinpol | 1043.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |
| rinpol | 1078.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |
| ripol | 1547.00 | | NIST Webbook |
| ripol | 1547.00 | | NIST Webbook |
| ripol | 1547.00 | | NIST Webbook |
| ripol | 1547.00 | | NIST Webbook |
| ripol | 1515.00 | | NIST Webbook |
| ripol | 1545.00 | | NIST Webbook |
| ripol | 1562.00 | | NIST Webbook |
| ripol | 1538.00 | | NIST Webbook |
| ripol | 1547.00 | | NIST Webbook |

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|---|---|---|---|
| tb | 550.03 | K | Joback Method |
| tc | 724.80 | K | Joback Method |
| tf | 282.90 | K | Joback Method |
| vc | 0.514 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 334.04 | J/mol×K | 550.03 | Joback Method |
| cpg | 345.30 | J/mol×K | 579.16 | Joback Method |
| cpg | 356.10 | J/mol×K | 608.29 | Joback Method |
| cpg | 366.45 | J/mol×K | 637.42 | Joback Method |
| cpg | 376.36 | J/mol×K | 666.54 | Joback Method |
| cpg | 385.82 | J/mol×K | 695.67 | Joback Method |
| cpg | 394.85 | J/mol×K | 724.80 | Joback Method |
| dvisc | 0.0249265 | Pa×s | 282.90 | Joback Method |
| dvisc | 0.0052844 | Pa×s | 327.42 | Joback Method |
| dvisc | 0.0016241 | Pa×s | 371.94 | Joback Method |
| dvisc | 0.0006423 | Pa×s | 416.46 | Joback Method |
| dvisc | 0.0003039 | Pa×s | 460.99 | Joback Method |
| dvisc | 0.0001640 | Pa×s | 505.51 | Joback Method |
| dvisc | 0.0000978 | Pa×s | 550.03 | Joback Method |

# 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=C10348477&Units=SI
**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

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