# Isoamyl lactate

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|---|---|
| **Other names:** | 3-Methylbutyl lactate |
| | 3-methylbutyl 2-hydroxypropanoate |
| | Isopentyl lactate |
| | Propanoic acid, 2-hydroxy-, 3-methylbutyl ester |
| | isopentyl 2-hydroxypropanoate |
| **Inchi:** | InChI=1S/C8H16O3/c1-6(2)4-5-11-8(10)7(3)9/h6-7,9H,4-5H2,1-3H3 |
| **InchiKey:** | CRORGGSWAKIXSA-UHFFFAOYSA-N |
| **Formula:** | C8H16O3 |
| **SMILES:** | CC(C)CCOC(=O)C(C)O |
| **Mol. weight [g/mol]:** | 160.21 |
| **CAS:** | 19329-89-6 |

# 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 | 1047.00 | | NIST Webbook |
| rinpol | 1047.00 | | NIST Webbook |
| ripol | 1583.00 | | NIST Webbook |
| ripol | 1614.00 | | NIST Webbook |
| ripol | 1572.00 | | NIST Webbook |
| ripol | 1614.00 | | NIST Webbook |
| ripol | 1619.00 | | NIST Webbook |
| ripol | 1580.00 | | NIST Webbook |
| ripol | 1558.00 | | NIST Webbook |
| ripol | 1570.00 | | NIST Webbook |
| ripol | 1615.00 | | NIST Webbook |
| ripol | 1560.00 | | NIST Webbook |
| ripol | 1547.00 | | NIST Webbook |
| ripol | 1572.00 | | NIST Webbook |
| ripol | 1558.00 | | NIST Webbook |

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| ripol | 1614.00 | | NIST Webbook |
| ripol | 1615.00 | | NIST Webbook |
| ripol | 1583.00 | | NIST Webbook |
| ripol | 1570.00 | | NIST Webbook |
| ripol | 1583.00 | | NIST Webbook |
| 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

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Heat Capacity, Density, Vapor Pressure, and Enthalpy of Vaporization of Isoamyl di Lactate:** | https://www.doi.org/10.1021/acs.jced.9b00209 |
| **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=C19329896&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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