# 2-Oxepanone

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| **Other names:** | .epsilon.-caprolactone |
| | 1,6-Hexanolide |
| | 1-Oxa-2-oxocycloheptane |
| | 2-Oxacycloheptanone |
| | 6-Caprolactone |
| | 6-Caprolactone monomer |
| | 6-Hexanalactone |
| | 6-Hexanolactone |
| | 6-Hexanolide |
| | 6-Hydroxyhexan-6-olide |
| | 6-Hydroxyhexanoic acid lactone |
| | Caprolactone |
| | E-caprolactone |
| | Epsilon-caprolactone |
| | Hexamethylene oxide, 2-oxo- |
| | Hexan-6-olide |
| | Hexanoic acid, 6-hydroxy-, lactone |
| | Hexanoic acid, 6-hydroxy-, «epsilon»-lactone |
| | Hexanoic acid, 6-hydroxy-, Â«epsilonÂ»-lactone |
| | Hexanoic acid, «epsilon»-lactone |
| | Hexanoic acid, Â«epsilonÂ»-lactone |
| | Placcel M |
| | oxepan-2-one |
| | «epsilon»-Caprolactone |
| | «epsilon»-Caprolactone monomer |
| | «epsilon»-Kaprolakton |
| | Â«epsilonÂ»-Caprolactone |
| | Â«epsilonÂ»-Caprolactone monomer |
| | Â«epsilonÂ»-Kaprolakton |
| **Inchi:** | InChI=1S/C6H10O2/c7-6-4-2-1-3-5-8-6/h1-5H2 |
| **InchiKey:** | PAPBSGBWRJIAAV-UHFFFAOYSA-N |
| **Formula:** | C6H10O2 |
| **SMILES:** | O=C1CCCCCO1 |
| **Mol. weight [g/mol]:** | 114.14 |
| **CAS:** | 502-44-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -189.01 | kJ/mol | Joback Method |
| hf | -396.00 ± 3.00 | kJ/mol | NIST Webbook |
| hfl | -458.00 ± 2.00 | kJ/mol | NIST Webbook |
| hfus | 7.45 | kJ/mol | Joback Method |
| hvap | 62.00 | kJ/mol | NIST Webbook |
| hvap | 62.00 ± 1.00 | kJ/mol | NIST Webbook |
| hvap | 62.00 ± 1.30 | kJ/mol | NIST Webbook |
| log10ws | -1.09 | | Crippen Method |
| logp | 1.104 | | Crippen Method |
| mcvol | 91.980 | ml/mol | McGowan Method |
| pc | 4414.96 | kPa | Joback Method |
| sl | 235.60 | J/mol×K | NIST Webbook |
| sl | 235.70 | J/mol×K | NIST Webbook |
| tb | 459.94 | K | Joback Method |
| tc | 695.47 | K | Joback Method |
| tf | 260.27 | K | Joback Method |
| tt | 272.13 ± 0.02 | K | NIST Webbook |
| tt | 271.83 ± 0.02 | K | NIST Webbook |
| vc | 0.326 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 256.71 | J/mol×K | 656.22 | Joback Method |
| cpg | 232.06 | J/mol×K | 577.71 | Joback Method |
| cpg | 218.67 | J/mol×K | 538.45 | Joback Method |
| cpg | 204.60 | J/mol×K | 499.20 | Joback Method |
| cpg | 189.87 | J/mol×K | 459.94 | Joback Method |
| cpg | 267.94 | J/mol×K | 695.47 | Joback Method |
| cpg | 244.74 | J/mol×K | 616.96 | Joback Method |
| cpl | 196.80 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 196.80 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0048852 | Pa×s | 303.15 | Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K |

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|---|---|---|---|---|
| dvisc | 0.0043237 | Pa×s | 308.15 | Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K |
| dvisc | 0.0038182 | Pa×s | 313.15 | Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K |
| dvisc | 0.0034203 | Pa×s | 318.15 | Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K |
| hfust | 13.82 | kJ/mol | 272.00 | NIST Webbook |
| hfust | 13.82 | kJ/mol | 271.83 | NIST Webbook |
| hfust | 13.82 | kJ/mol | 272.13 | NIST Webbook |
| hvapt | 54.00 ± 0.20 | kJ/mol | 415.50 | NIST Webbook |
| pvap | 0.04 | kPa | 283.20 | Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone |
| pvap | 0.34 | kPa | 323.10 | Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone |
| pvap | 0.21 | kPa | 313.10 | Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone |
| pvap | 0.13 | kPa | 302.90 | Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone |

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|---|---|---|---|---|
| pvap | 0.08 | kPa | 292.90 | Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone |
| pvap | 0.52 | kPa | 333.20 | Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone |
| pvap | 0.77 | kPa | 343.20 | Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone |
| sfust | 50.90 | J/mol×K | 271.83 | NIST Webbook |
| sfust | 50.90 | J/mol×K | 272.13 | NIST Webbook |
| speedsl | 1567.76 | m/s | 293.15 | A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones |
| speedsl | 1548.28 | m/s | 298.15 | A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones |
| speedsl | 1528.99 | m/s | 303.15 | A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones |
| speedsl | 1509.98 | m/s | 308.15 | A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones |
| speedsl | 1491.20 | m/s | 313.15 | A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones |

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| speedsl | 1472.68 | m/s | 318.15 | A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones |
| speedsl | 1454.52 | m/s | 323.15 | A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 370.20 | K | 2.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 3.47420e+01 |
| Coeff. B | -1.27202e+04 |
| Coeff. C | -4.53800e+00 |
| Temperature range (K), min. | 373.73 |
| Temperature range (K), max. | 436.75 |

# Sources

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|---|---|
| **Measurement and Correlation for Solubilities of Adipic Acid in Acetic Acid + ε-Caprolactone Mixtures and Cyclohexanone + ε-Caprolactones Mixtures:** | https://www.doi.org/10.1021/acs.jced.6b00177 |
| **High Pressure Phase Equilibrium Data for the Ternary System Containing Cyclohexanone, ε-Caprolactone, and Dichloromethane:** | https://www.doi.org/10.1021/acs.jced.8b01017 |
| **ClinnaqMethod:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Vapour pressure data of epsilon-Caprolactone:** | https://www.doi.org/10.1016/j.jct.2007.09.008 |
| **e-caprolactone, d-hexalactone, and ε-caprolactone:** | http://link.springer.com/article/10.1007/BF02311772 |
| **McGowan Method:** | |

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| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C502443&Units=SI |
| **Phase behaviour of binary systems of lactones in carbon dioxide:** | https://www.doi.org/10.1016/j.jct.2009.07.003 |
| **A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered ring lactones:** | https://www.doi.org/10.1016/j.jct.2016.12.032 |
| **Measurement and Correlation for Solubilities of Succinic Acid and Glutaric Acid in ε-Caprolactone + Acetic Acid Mixtures and ε-Caprolactone + Cyclohexanone Mixtures:** | https://www.doi.org/10.1021/acs.jced.7b00660 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K:** | https://www.doi.org/10.1016/j.jct.2008.05.004 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **sfust:** | Entropy of fusion at a given temperature |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **speedsl:** | Speed of sound in fluid |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |