

# Propanoic acid, 2-hydroxy-, ethyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | (+)-ethyl 2-hydroxypropionate<br>(+)-ethyl lactate<br>(. +/-)-Ethyl lactate<br>(S)-(-)-ethyl lactate<br>(dl) ethyl lactate<br>2-Hydroxypropanoic acid ethyl ester<br>Actylol<br>Acytol<br>DL-ethyl 2-hydroxypropionate<br>DL-ethyl lactate<br>Ethyl 2-hydroxypropionate<br>Ethyl ester of lactic acid<br>Ethyl lactate<br>Ethyl racemic-lactate<br>Ethyl «alpha»-hydroxypropionate<br>Ethyl «alpha»-hydroxypropionate<br>Ethylester kyseliny mlecne<br>Eusolvan<br>L-ethyl 2-hydroxypropanoate<br>L-ethyl lactate<br>L-lactic acid, ethyl ester<br>Lactate d'ethyle<br>Lactic acid, ethyl ester<br>NSC 8850<br>Solactol<br>UN 1192<br>ethyl 2-hydroxypropanoate |
| <b>Inchi:</b>               | InChI=1S/C5H10O3/c1-3-8-5(7)4(2)6/h4,6H,3H2,1-2H3   |
| <b>InchiKey:</b>            | LZCLXQDLBQLTDK-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C5H10O3   |
| <b>SMILES:</b>              | CCOC(=O)C(C)O   |
| <b>Mol. weight [g/mol]:</b> | 118.13  |
| <b>CAS:</b>                 | 97-64-3   |

## 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  |
| rinpol  | 821.00  |  |        | NIST Webbook   |
| rinpol  | 798.00  |  |        | NIST Webbook   |
| rinpol  | 799.00  |  |        | NIST Webbook   |
| rinpol  | 801.00  |  |        | NIST Webbook   |
| rinpol  | 813.00  |  |        | NIST Webbook   |
| rinpol  | 815.00  |  |        | NIST Webbook   |
| rinpol  | 815.00  |  |        | NIST Webbook   |
| rinpol  | 797.00  |  |        | NIST Webbook   |
| rinpol  | 815.00  |  |        | NIST Webbook   |
| rinpol  | 789.00  |  |        | NIST Webbook   |
| rinpol  | 836.00  |  |        | NIST Webbook   |
| rinpol  | 764.00  |  |        | NIST Webbook   |
| rinpol  | 787.00  |  |        | NIST Webbook   |
| rinpol  | 832.00  |  |        | NIST Webbook   |
| rinpol  | 815.00  |  |        | NIST Webbook   |
| rinpol  | 797.00  |  |        | NIST Webbook   |
| rinpol  | 821.00  |  |        | NIST Webbook   |
| rinpol  | 798.00  |  |        | NIST Webbook   |
| rinpol  | 788.00  |  |        | NIST Webbook   |
| rinpol  | 798.00  |  |        | NIST Webbook   |
| rinpol  | 813.00  |  |        | NIST Webbook   |
| rinpol  | 801.00  |  |        | NIST Webbook   |
| rinpol  | 803.00  |  |        | NIST Webbook   |
| rinpol  | 764.00  |  |        | NIST Webbook   |
| rinpol  | 821.00  |  |        | NIST Webbook   |
| rinpol  | 801.00  |  |        | NIST Webbook   |
| rinpol  | 803.00  |  |        | NIST Webbook   |
| rinpol  | 787.00  |  |        | NIST Webbook   |
| rinpol  | 787.00  |  |        | NIST Webbook   |
| rinpol  | 806.00  |  |        | NIST Webbook   |
| rinpol  | 803.00  |  |        | NIST Webbook   |
| rinpol  | 826.00  |  |        | NIST Webbook   |
| ripol   | 1331.00 |  |        | NIST Webbook   |
| ripol   | 1309.00 |  |        | NIST Webbook   |
| ripol   | 1312.00 |  |        | NIST Webbook   |
| ripol   | 1340.00 |  |        | NIST Webbook   |

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|-------|---------|--------------|
| ripol | 1352.00 | NIST Webbook |
| ripol | 1353.00 | NIST Webbook |
| ripol | 1342.00 | NIST Webbook |
| ripol | 1329.00 | NIST Webbook |
| ripol | 1333.00 | NIST Webbook |
| ripol | 1333.00 | NIST Webbook |
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| ripol | 1347.00 | NIST Webbook |
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| ripol | 1353.00 | NIST Webbook |
| ripol | 1372.00 | NIST Webbook |
| ripol | 1356.00 | NIST Webbook |
| ripol | 1362.00 | NIST Webbook |
| ripol | 1338.00 | NIST Webbook |
| ripol | 1334.00 | NIST Webbook |
| ripol | 1334.00 | NIST Webbook |
| ripol | 1334.00 | NIST Webbook |
| ripol | 1349.00 | NIST Webbook |
| ripol | 1371.00 | NIST Webbook |
| ripol | 1349.00 | NIST Webbook |
| ripol | 1349.00 | NIST Webbook |
| ripol | 1356.00 | NIST Webbook |
| ripol | 1362.00 | NIST Webbook |
| ripol | 1331.00 | NIST Webbook |
| ripol | 1337.00 | NIST Webbook |
| ripol | 1312.00 | NIST Webbook |
| ripol | 1367.00 | NIST Webbook |
| ripol | 1355.00 | NIST Webbook |
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| ripol | 1334.00 | NIST Webbook |
| ripol | 1339.00 | NIST Webbook |
| ripol | 1353.00 | NIST Webbook |

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|-------|---------|----------------------|---------------|
| ripol | 1354.00 |                      | NIST Webbook  |
| ripol | 1353.00 |                      | NIST Webbook  |
| ripol | 1356.00 |                      | NIST Webbook  |
| ripol | 1340.00 |                      | NIST Webbook  |
| ripol | 1363.00 |                      | NIST Webbook  |
| ripol | 1353.00 |                      | NIST Webbook  |
| ripol | 1363.00 |                      | NIST Webbook  |
| ripol | 1348.00 |                      | NIST Webbook  |
| ripol | 1348.00 |                      | NIST Webbook  |
| ripol | 1321.00 |                      | NIST Webbook  |
| ripol | 1363.00 |                      | NIST Webbook  |
| ripol | 1341.00 |                      | NIST Webbook  |
| ripol | 1349.00 |                      | NIST Webbook  |
| ripol | 1364.00 |                      | NIST Webbook  |
| ripol | 1348.00 |                      | NIST Webbook  |
| ripol | 1334.00 |                      | NIST Webbook  |
| ripol | 1338.00 |                      | NIST Webbook  |
| ripol | 1353.00 |                      | NIST Webbook  |
| ripol | 1338.00 |                      | NIST Webbook  |
| ripol | 1371.00 |                      | NIST Webbook  |
| ripol | 1339.00 |                      | NIST Webbook  |
| ripol | 1330.00 |                      | NIST Webbook  |
| ripol | 1356.00 |                      | NIST Webbook  |
| ripol | 1358.00 |                      | NIST Webbook  |
| ripol | 1312.00 |                      | NIST Webbook  |
| ripol | 1342.00 |                      | NIST Webbook  |
| ripol | 1347.00 |                      | NIST Webbook  |
| ripol | 1316.00 |                      | NIST Webbook  |
| ripol | 1353.00 |                      | NIST Webbook  |
| ripol | 1348.00 |                      | NIST Webbook  |
| tb    | 481.83  | K                    | Joback Method |
| tc    | 657.66  | K                    | Joback Method |
| tf    | 264.09  | K                    | Joback Method |
| vc    | 0.352   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 248.43 | J/molxK | 657.66          | Joback Method |
| cpg           | 212.77 | J/molxK | 511.13          | Joback Method |
| cpg           | 220.46 | J/molxK | 540.44          | Joback Method |

|       |           |         |        |  |
|-------|-----------|---------|--------|--|
| cpg   | 227.87    | J/mol×K | 569.74 | Joback Method  |
| cpg   | 235.00    | J/mol×K | 599.05 | Joback Method  |
| cpg   | 241.86    | J/mol×K | 628.35 | Joback Method  |
| cpg   | 204.80    | J/mol×K | 481.83 | Joback Method  |
| dvisc | 0.0023980 | Paxs    | 298.15 | Densities and Viscosities for Binary Mixtures of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K |
| dvisc | 0.0018630 | Paxs    | 308.15 | Densities and Viscosities for Binary Mixtures of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K |
| dvisc | 0.0014940 | Paxs    | 318.15 | Densities and Viscosities for Binary Mixtures of Ethyl Lactate with Methacrylic Acid, Benzyl Methacrylate, and 2-Hydroxyethyl Methacrylate at (298.15, 308.15, and 318.15) K |
| hvapt | 49.20     | kJ/mol  | 367.00 | NIST Webbook   |
| hvapt | 51.30     | kJ/mol  | 375.50 | NIST Webbook   |
| pvap  | 0.13      | kPa     | 287.60 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods                                  |

|      |      |     |        |   |
|------|------|-----|--------|---|
| pvap | 0.05 | kPa | 276.60 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.07 | kPa | 279.60 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.07 | kPa | 281.40 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.09 | kPa | 283.60 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.10 | kPa | 284.60 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |

|      |      |     |        |   |
|------|------|-----|--------|---|
| pvap | 0.10 | kPa | 285.80 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.13 | kPa | 287.60 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.04 | kPa | 274.60 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.13 | kPa | 288.40 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.15 | kPa | 290.20 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |

|      |      |     |        |   |
|------|------|-----|--------|---|
| pvap | 0.15 | kPa | 290.30 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.16 | kPa | 291.10 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.19 | kPa | 293.50 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.24 | kPa | 296.40 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.28 | kPa | 298.50 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |



|      |      |     |        |   |
|------|------|-----|--------|---|
| pvap | 0.37 | kPa | 301.50 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.38 | kPa | 302.50 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.45 | kPa | 304.50 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.48 | kPa | 305.30 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |
| pvap | 0.53 | kPa | 307.20 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods |

|      |         |     |        |  |
|------|---------|-----|--------|--|
| pvap | 0.58    | kPa | 308.20 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods                              |
| pvap | 0.63    | kPa | 310.10 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods                              |
| pvap | 0.63    | kPa | 310.10 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods                              |
| pvap | 0.69    | kPa | 311.30 | Renewable platform chemicals: Evaluation of thermochemical data of alkyl lactates with complementary experimental and computational methods                              |
| rfi  | 1.41290 |     | 293.15 | Vapor liquid equilibria and excess volumes of the binary systems ethanol + ethyl lactate, isopropanol + isopropyl lactate and n-butanol + n-butyl lactate at 101.325 kPa |

|      |         |       |        |  |
|------|---------|-------|--------|--|
| rfi  | 1.41050 |       | 298.15 | Density, Refractive Index, Speed of Sound at 298.15 K, and Vapor-Liquid Equilibria at 101.3 kPa for Binary Mixtures of Ethyl Acetate + Ethyl Lactate and Methyl Acetate + Ethyl Lactate  |
| rfi  | 1.41057 |       | 298.15 | Isobaric Vapor Liquid Equilibrium of 3-Methyl-1-butanol + Ethyl Lactate and 1-Pentanol + Ethyl Lactate at (13.0 and 101.3) kPa   |
| rhoI | 1039.28 | kg/m3 | 288.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |
| rhoI | 1033.84 | kg/m3 | 293.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |

|      |         |       |        |  |
|------|---------|-------|--------|--|
| rho1 | 1028.39 | kg/m3 | 298.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |
| rho1 | 1022.92 | kg/m3 | 303.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |
| rho1 | 1017.42 | kg/m3 | 308.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |

|      |         |       |        |  |
|------|---------|-------|--------|--|
| rho1 | 1011.90 | kg/m3 | 313.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |
| rho1 | 1006.36 | kg/m3 | 318.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |
| rho1 | 1000.79 | kg/m3 | 323.15 | Volumetric and viscometric behavior of the binary systems ethyl lactate + 1,2- propanediol, + 1,3-propanediol, + tetrahydrofuran and + tetraethylene glycol dimethyl ether. New UNIFAC-VISCO and ASOG-VISCO parameters determination |

|      |         |       |        |  |
|------|---------|-------|--------|--|
| rho1 | 1028.39 | kg/m3 | 298.15 | Experimental measurements and modelling of volumetric properties, refractive index and viscosity of binary systems of ethyl lactate with methyl ethyl ketone, toluene and n-methyl-2-pyrrolidone at 288.15 323.15 K and atmospheric pressure. New UNIFAC VISCO and ASOG VISCO interaction parameters |
| rho1 | 1028.08 | kg/m3 | 298.15 | Vapor-liquid equilibria of binary and ternary mixtures containing ethyl lactate and effect of ethyl lactate as entrainer   |
| rho1 | 1028.37 | kg/m3 | 298.15 | Self-aggregation of liquids from biomass in aqueous solution   |
| rho1 | 1050.05 | kg/m3 | 278.15 | Thermophysical Properties of Lactates  |
| rho1 | 1047.37 | kg/m3 | 280.65 | Thermophysical Properties of Lactates  |
| rho1 | 1044.68 | kg/m3 | 283.15 | Thermophysical Properties of Lactates  |
| rho1 | 1041.96 | kg/m3 | 285.65 | Thermophysical Properties of Lactates  |
| rho1 | 1039.26 | kg/m3 | 288.15 | Thermophysical Properties of Lactates  |
| rho1 | 1036.54 | kg/m3 | 290.65 | Thermophysical Properties of Lactates  |
| rho1 | 1033.82 | kg/m3 | 293.15 | Thermophysical Properties of Lactates  |
| rho1 | 1031.09 | kg/m3 | 295.65 | Thermophysical Properties of Lactates  |
| rho1 | 1028.37 | kg/m3 | 298.15 | Thermophysical Properties of Lactates  |

|      |         |       |        |   |
|------|---------|-------|--------|---|
| rho1 | 1028.08 | kg/m3 | 298.15 | Separation Effects of Renewable Solvent Ethyl Lactate on the Vapor Liquid Equilibria of the Methanol + Dimethyl Carbonate Azeotropic System |
| rho1 | 1022.89 | kg/m3 | 303.15 | Thermophysical Properties of Lactates   |
| rho1 | 1020.15 | kg/m3 | 305.65 | Thermophysical Properties of Lactates   |
| rho1 | 1017.40 | kg/m3 | 308.15 | Thermophysical Properties of Lactates   |
| rho1 | 1014.64 | kg/m3 | 310.65 | Thermophysical Properties of Lactates   |
| rho1 | 1011.88 | kg/m3 | 313.15 | Thermophysical Properties of Lactates   |
| rho1 | 1009.12 | kg/m3 | 315.65 | Thermophysical Properties of Lactates   |
| rho1 | 1006.34 | kg/m3 | 318.15 | Thermophysical Properties of Lactates   |
| rho1 | 1003.57 | kg/m3 | 320.65 | Thermophysical Properties of Lactates   |
| rho1 | 1000.78 | kg/m3 | 323.15 | Thermophysical Properties of Lactates   |
| rho1 | 997.99  | kg/m3 | 325.65 | Thermophysical Properties of Lactates   |
| rho1 | 995.19  | kg/m3 | 328.15 | Thermophysical Properties of Lactates   |
| rho1 | 992.39  | kg/m3 | 330.65 | Thermophysical Properties of Lactates   |
| rho1 | 989.58  | kg/m3 | 333.15 | Thermophysical Properties of Lactates   |
| rho1 | 986.76  | kg/m3 | 335.65 | Thermophysical Properties of Lactates   |
| rho1 | 983.94  | kg/m3 | 338.15 | Thermophysical Properties of Lactates   |

|         |         |                   |        |  |
|---------|---------|-------------------|--------|--|
| rhoI    | 1025.63 | kg/m <sup>3</sup> | 300.65 | Thermophysical Properties of Lactates  |
| speedsl | 1261.10 | m/s               | 303.15 | Densities, speed of sound, and IR studies of Ethyl lactate with 2-alkoxyethanols at different temperatures |
| speedsl | 1243.80 | m/s               | 308.15 | Densities, speed of sound, and IR studies of Ethyl lactate with 2-alkoxyethanols at different temperatures |
| speedsl | 1224.80 | m/s               | 313.15 | Densities, speed of sound, and IR studies of Ethyl lactate with 2-alkoxyethanols at different temperatures |
| speedsl | 1206.90 | m/s               | 318.15 | Densities, speed of sound, and IR studies of Ethyl lactate with 2-alkoxyethanols at different temperatures |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.89834e+01                   |
| Coeff. B                    | -6.73793e+03                  |
| Coeff. C                    | 4.18990e+01                   |
| Temperature range (K), min. | 318.50                        |
| Temperature range (K), max. | 450.93                        |

## Datasets



## Mass density, kg/m<sup>3</sup>

| Temperature, K - Liquid | Pressure, kPa - Liquid | Mass density, kg/m <sup>3</sup> - Liquid |
|-------------------------|------------------------|--|
| 283.15                  | 100.00                 | 1045.06                                  |
| 288.15                  | 100.00                 | 1039.64                                  |
| 293.15                  | 100.00                 | 1034.25                                  |
| 298.15                  | 100.00                 | 1028.78                                  |
| 303.15                  | 100.00                 | 1023.32                                  |
| 308.15                  | 100.00                 | 1017.84                                  |
| 313.15                  | 100.00                 | 1012.33                                  |
| 318.15                  | 100.00                 | 1006.72                                  |
| 323.15                  | 100.00                 | 1001.23                                  |
| 328.15                  | 100.00                 | 995.54                                   |
| 333.15                  | 100.00                 | 989.91                                   |
| 338.15                  | 100.00                 | 984.3                                    |
| 283.15                  | 2500.00                | 1046.77                                  |
| 288.15                  | 2500.00                | 1041.39                                  |
| 293.15                  | 2500.00                | 1036.05                                  |
| 298.15                  | 2500.00                | 1030.66                                  |
| 303.15                  | 2500.00                | 1025.21                                  |
| 308.15                  | 2500.00                | 1019.82                                  |
| 313.15                  | 2500.00                | 1014.31                                  |
| 318.15                  | 2500.00                | 1008.86                                  |
| 323.15                  | 2500.00                | 1003.36                                  |
| 328.15                  | 2500.00                | 997.8                                    |
| 333.15                  | 2500.00                | 992.19                                   |
| 338.15                  | 2500.00                | 986.71                                   |
| 283.15                  | 5000.00                | 1048.51                                  |
| 288.15                  | 5000.00                | 1043.21                                  |
| 293.15                  | 5000.00                | 1037.86                                  |
| 298.15                  | 5000.00                | 1032.56                                  |
| 303.15                  | 5000.00                | 1027.24                                  |
| 308.15                  | 5000.00                | 1021.87                                  |
| 313.15                  | 5000.00                | 1016.42                                  |
| 318.15                  | 5000.00                | 1011.01                                  |
| 323.15                  | 5000.00                | 1005.56                                  |
| 328.15                  | 5000.00                | 1000.11                                  |
| 333.15                  | 5000.00                | 994.55                                   |
| 338.15                  | 5000.00                | 989.18                                   |
| 283.15                  | 7500.00                | 1050.24                                  |
| 288.15                  | 7500.00                | 1044.99                                  |
| 293.15                  | 7500.00                | 1039.7                                   |

|        |          |         |
|--------|----------|---------|
| 298.15 | 7500.00  | 1034.43 |
| 303.15 | 7500.00  | 1029.11 |
| 308.15 | 7500.00  | 1023.84 |
| 313.15 | 7500.00  | 1018.41 |
| 318.15 | 7500.00  | 1013.1  |
| 323.15 | 7500.00  | 1007.68 |
| 328.15 | 7500.00  | 1002.34 |
| 333.15 | 7500.00  | 996.87  |
| 338.15 | 7500.00  | 991.49  |
| 283.15 | 10000.00 | 1051.88 |
| 288.15 | 10000.00 | 1046.74 |
| 293.15 | 10000.00 | 1041.5  |
| 298.15 | 10000.00 | 1036.23 |
| 303.15 | 10000.00 | 1031.0  |
| 308.15 | 10000.00 | 1025.7  |
| 313.15 | 10000.00 | 1020.39 |
| 318.15 | 10000.00 | 1015.13 |
| 323.15 | 10000.00 | 1009.78 |
| 328.15 | 10000.00 | 1004.46 |
| 333.15 | 10000.00 | 999.06  |
| 338.15 | 10000.00 | 993.65  |
| 283.15 | 20000.00 | 1058.39 |
| 288.15 | 20000.00 | 1053.28 |
| 293.15 | 20000.00 | 1048.3  |
| 298.15 | 20000.00 | 1043.21 |
| 303.15 | 20000.00 | 1038.26 |
| 308.15 | 20000.00 | 1033.08 |
| 313.15 | 20000.00 | 1027.93 |
| 318.15 | 20000.00 | 1022.87 |
| 323.15 | 20000.00 | 1017.76 |
| 328.15 | 20000.00 | 1012.65 |
| 333.15 | 20000.00 | 1007.62 |
| 338.15 | 20000.00 | 1002.34 |
| 283.15 | 30000.00 | 1064.45 |
| 288.15 | 30000.00 | 1059.46 |
| 293.15 | 30000.00 | 1054.58 |
| 298.15 | 30000.00 | 1049.76 |
| 303.15 | 30000.00 | 1044.91 |
| 308.15 | 30000.00 | 1039.92 |
| 313.15 | 30000.00 | 1034.97 |
| 318.15 | 30000.00 | 1030.04 |
| 323.15 | 30000.00 | 1025.13 |
| 328.15 | 30000.00 | 1020.17 |
| 333.15 | 30000.00 | 1015.4  |

|        |          |         |
|--------|----------|---------|
| 338.15 | 30000.00 | 1010.27 |
| 283.15 | 40000.00 | 1070.13 |
| 288.15 | 40000.00 | 1065.24 |
| 293.15 | 40000.00 | 1060.54 |
| 298.15 | 40000.00 | 1055.69 |
| 303.15 | 40000.00 | 1051.19 |
| 308.15 | 40000.00 | 1046.28 |
| 313.15 | 40000.00 | 1041.52 |
| 318.15 | 40000.00 | 1036.74 |
| 323.15 | 40000.00 | 1031.99 |
| 328.15 | 40000.00 | 1027.16 |
| 333.15 | 40000.00 | 1022.5  |
| 338.15 | 40000.00 | 1017.75 |
| 283.15 | 50000.00 | 1075.5  |
| 288.15 | 50000.00 | 1070.74 |
| 293.15 | 50000.00 | 1066.26 |
| 298.15 | 50000.00 | 1061.53 |
| 303.15 | 50000.00 | 1056.95 |
| 308.15 | 50000.00 | 1052.19 |
| 313.15 | 50000.00 | 1047.69 |
| 318.15 | 50000.00 | 1042.96 |
| 323.15 | 50000.00 | 1038.42 |
| 328.15 | 50000.00 | 1033.75 |
| 333.15 | 50000.00 | 1029.24 |
| 338.15 | 50000.00 | 1024.55 |
| 283.15 | 60000.00 | 1080.55 |
| 288.15 | 60000.00 | 1076.04 |
| 293.15 | 60000.00 | 1071.55 |
| 298.15 | 60000.00 | 1066.96 |
| 303.15 | 60000.00 | 1062.52 |
| 308.15 | 60000.00 | 1057.98 |
| 313.15 | 60000.00 | 1053.46 |
| 318.15 | 60000.00 | 1048.96 |
| 323.15 | 60000.00 | 1044.49 |
| 328.15 | 60000.00 | 1039.99 |
| 333.15 | 60000.00 | 1035.71 |
| 338.15 | 60000.00 | 1031.04 |

Reference

<https://www.doi.org/10.1016/j.jct.2012.11.002>

| Temperature, K | Pressure, kPa | Mass density, kg/m <sup>3</sup> |
|----------------|---------------|---------------------------------|
| 298.15         | 100.00        | 1028.45                         |



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[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>pvap:</b>    | Vapor pressure                                  |
| <b>rfi:</b>     | Refractive Index                                |
| <b>rhoL:</b>    | Liquid Density                                  |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>speedsl:</b> | Speed of sound in fluid                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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