

# Dodecanoic acid, ethyl ester

|                      |                                                                         |
|----------------------|-------------------------------------------------------------------------|
| Other names:         | Ethyl dodecanoate                                                       |
|                      | Ethyl dodecylate                                                        |
|                      | Ethyl ester dodecanoic acid                                             |
|                      | Ethyl ester of dodecanoic acid                                          |
|                      | Ethyl laurate                                                           |
|                      | Ethyl laurinate                                                         |
|                      | Ethyl n-dodecanoate                                                     |
|                      | Ethyl n-dodecanote                                                      |
|                      | Lauric acid, ethyl ester                                                |
| Inchi:               | InChI=1S/C14H28O2/c1-3-5-6-7-8-9-10-11-12-13-14(15)16-4-2/h3-13H2,1-2H3 |
| InchiKey:            | MMXKVMNBHPAILY-UHFFFAOYSA-N                                             |
| Formula:             | C14H28O2                                                                |
| SMILES:              | CCCCCCCCCCCC(=O)OCC                                                     |
| Mol. weight [g/mol]: | 228.37                                                                  |
| CAS:                 | 106-33-2                                                                |

## Physical Properties

| Property code | Value           | Unit   | Source                                                                                          |
|---------------|-----------------|--------|-------------------------------------------------------------------------------------------------|
| chl           | -8778.00 ± 1.00 | kJ/mol | NIST Webbook                                                                                    |
| gf            | -166.92         | kJ/mol | Joback Method                                                                                   |
| hf            | -577.09         | kJ/mol | Joback Method                                                                                   |
| hfus          | 39.83           | kJ/mol | Solid liquid equilibrium in ternary mixtures of ethyl oleate, ethyl laurate and ethyl palmitate |
| hvap          | 80.00           | kJ/mol | NIST Webbook                                                                                    |
| log10ws       | -4.55           |        | Crippen Method                                                                                  |
| logp          | 4.470           |        | Crippen Method                                                                                  |
| mcvol         | 215.560         | ml/mol | McGowan Method                                                                                  |
| pc            | 1579.71         | kPa    | Joback Method                                                                                   |
| rinpol        | 1558.00         |        | NIST Webbook                                                                                    |
| rinpol        | 1579.00         |        | NIST Webbook                                                                                    |
| rinpol        | 1578.00         |        | NIST Webbook                                                                                    |
| rinpol        | 1579.00         |        | NIST Webbook                                                                                    |
| rinpol        | 1578.00         |        | NIST Webbook                                                                                    |
| rinpol        | 1582.00         |        | NIST Webbook                                                                                    |
| rinpol        | 1581.00         |        | NIST Webbook                                                                                    |
| rinpol        | 1593.00         |        | NIST Webbook                                                                                    |

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|--------|---------|--------------|
| rinpol | 1597.00 | NIST Webbook |
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| rinpol | 1566.00 | NIST Webbook |
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| rinpol | 1577.00 | NIST Webbook |
| rinpol | 1577.00 | NIST Webbook |
| rinpol | 1581.00 | NIST Webbook |
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| rinpol | 1598.00 | NIST Webbook |
| rinpol | 1595.00 | NIST Webbook |
| rinpol | 1590.00 | NIST Webbook |
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| rinpol | 1578.00 | NIST Webbook |

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| rinpol | 1592.00 | NIST Webbook |
| rinpol | 1603.00 | NIST Webbook |
| rinpol | 1603.00 | NIST Webbook |
| rinpol | 1595.00 | NIST Webbook |
| rinpol | 1595.00 | NIST Webbook |
| rinpol | 1595.00 | NIST Webbook |
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| rinpol | 1597.00 | NIST Webbook |
| rinpol | 1597.00 | NIST Webbook |
| rinpol | 1583.00 | NIST Webbook |
| rinpol | 1595.00 | NIST Webbook |
| rinpol | 1597.00 | NIST Webbook |
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| rinpol | 1579.00 | NIST Webbook |
| rinpol | 1576.00 | NIST Webbook |
| rinpol | 1577.00 | NIST Webbook |
| rinpol | 267.60  | NIST Webbook |
| rinpol | 1593.00 | NIST Webbook |
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| ripol  | 1839.00 | NIST Webbook |
| ripol  | 1850.00 | NIST Webbook |
| ripol  | 1828.00 | NIST Webbook |
| ripol  | 1836.00 | NIST Webbook |
| ripol  | 1865.00 | NIST Webbook |
| ripol  | 1866.00 | NIST Webbook |

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| ripol | 1826.00       |   | NIST Webbook  |
| ripol | 1830.00       |   | NIST Webbook  |
| ripol | 1820.00       |   | NIST Webbook  |
| ripol | 1829.00       |   | NIST Webbook  |
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| ripol | 1826.00       |   | NIST Webbook  |
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| ripol | 1849.00       |   | NIST Webbook  |
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| ripol | 1818.00       |   | NIST Webbook  |
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| ripol | 1826.00       |   | NIST Webbook  |
| ripol | 1850.00       |   | NIST Webbook  |
| ripol | 1826.00       |   | NIST Webbook  |
| ripol | 1848.00       |   | NIST Webbook  |
| ripol | 1843.00       |   | NIST Webbook  |
| tb    | 448.00 ± 2.00 | K | NIST Webbook  |
| tb    | 463.00 ± 1.50 | K | NIST Webbook  |
| tc    | 764.02        | K | Joback Method |

|    |               |         |                                                                                                                          |
|----|---------------|---------|--------------------------------------------------------------------------------------------------------------------------|
| tf | 272.20        | K       | High pressure solid-liquid equilibrium of fatty acid ethyl esters binary systems                                         |
| tf | 273.20        | K       | Solid-liquid equilibrium in ternary mixtures of ethyl laurate, ethyl palmitate and ethyl stearate                        |
| tf | 262.50 ± 0.20 | K       | NIST Webbook                                                                                                             |
| tt | 273.00        | K       | Influence of Additives (Isoamyl Laurate or Isoamyl Nonanoate) in the Solid-Liquid Equilibrium of Fatty Acid Ethyl Esters |
| vc | 0.844         | m3/kmol | Joback Method                                                                                                            |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source                                                          |
|---------------|-----------|---------|-----------------|-----------------------------------------------------------------|
| cpg           | 567.02    | J/mol×K | 596.01          | Joback Method                                                   |
| cpg           | 600.10    | J/mol×K | 652.01          | Joback Method                                                   |
| cpg           | 615.63    | J/mol×K | 680.02          | Joback Method                                                   |
| cpg           | 630.49    | J/mol×K | 708.02          | Joback Method                                                   |
| cpg           | 644.71    | J/mol×K | 736.02          | Joback Method                                                   |
| cpg           | 658.29    | J/mol×K | 764.02          | Joback Method                                                   |
| cpg           | 583.90    | J/mol×K | 624.01          | Joback Method                                                   |
| dvisc         | 0.0013486 | Pa×s    | 343.15          | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters |
| dvisc         | 0.0015703 | Pa×s    | 333.15          | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters |
| dvisc         | 0.0017037 | Pa×s    | 328.15          | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters |
| dvisc         | 0.0018531 | Pa×s    | 323.15          | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters |
| dvisc         | 0.0020240 | Pa×s    | 318.15          | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters |
| dvisc         | 0.0012543 | Pa×s    | 348.15          | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters |

|       |           |        |        |                                                                                                      |
|-------|-----------|--------|--------|------------------------------------------------------------------------------------------------------|
| dvisc | 0.0024455 | Pa×s   | 308.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0027073 | Pa×s   | 303.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0030152 | Pa×s   | 298.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0038135 | Pa×s   | 288.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0043353 | Pa×s   | 283.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0011708 | Pa×s   | 353.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0014529 | Pa×s   | 338.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0033797 | Pa×s   | 293.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| dvisc | 0.0022198 | Pa×s   | 313.15 | Densities and Viscosities of Fatty Acid Methyl and Ethyl Esters                                      |
| hfust | 9.31      | kJ/mol | 271.50 | NIST Webbook                                                                                         |
| hfust | 9.31      | kJ/mol | 271.50 | NIST Webbook                                                                                         |
| hfust | 9.31      | kJ/mol | 271.45 | NIST Webbook                                                                                         |
| hvapt | 67.20     | kJ/mol | 410.50 | NIST Webbook                                                                                         |
| pvap  | 9.33      | kPa    | 464.35 | Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry             |
| pvap  | 0.03      | kPa    | 351.88 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |

|      |      |     |        |                                                                                                      |
|------|------|-----|--------|------------------------------------------------------------------------------------------------------|
| pvap | 0.12 | kPa | 372.12 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 0.23 | kPa | 382.17 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 8.00 | kPa | 462.44 | Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry             |
| pvap | 1.70 | kPa | 422.15 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 2.65 | kPa | 432.26 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 3.99 | kPa | 442.27 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 5.80 | kPa | 452.31 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 8.49 | kPa | 462.43 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 6.67 | kPa | 456.47 | Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry             |

|      |          |     |        |                                                                                                      |
|------|----------|-----|--------|------------------------------------------------------------------------------------------------------|
| pvap | 0.40     | kPa | 392.24 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 5.33     | kPa | 451.05 | Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry             |
| pvap | 4.00     | kPa | 443.41 | Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry             |
| pvap | 2.67     | kPa | 432.13 | Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry             |
| pvap | 1.33     | kPa | 420.05 | Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry             |
| pvap | 0.67     | kPa | 402.20 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 0.07     | kPa | 362.10 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| pvap | 1.83e-03 | kPa | 313.10 | Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE) Components of Biodiesel |
| rfi  | 1.42547  |     | 308.15 | Thermophysical properties of fatty acid methyl and ethyl esters                                      |

|     |         |        |                                                                 |
|-----|---------|--------|-----------------------------------------------------------------|
| rfi | 1.42125 | 318.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.42335 | 313.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.41707 | 328.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.41501 | 333.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.41295 | 338.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.41090 | 343.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.40886 | 348.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.40684 | 353.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.42961 | 298.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.43169 | 293.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.43375 | 288.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.43583 | 283.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.43791 | 278.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.40479 | 358.15 | Thermophysical properties of fatty acid methyl and ethyl esters |
| rfi | 1.41915 | 323.15 | Thermophysical properties of fatty acid methyl and ethyl esters |

|      |         |       |        |                                                                                                              |  |
|------|---------|-------|--------|--------------------------------------------------------------------------------------------------------------|--|
| rfi  | 1.42755 |       | 303.15 | Thermophysical properties of fatty acid methyl and ethyl esters                                              |  |
| rhoI | 858.19  | kg/m3 | 298.15 | Measurement and correlation of density and viscosity of n-hexadecane with three fatty acid ethyl esters      |  |
| rhoI | 854.30  | kg/m3 | 303.15 | Measurement and correlation of density and viscosity of n-hexadecane with three fatty acid ethyl esters      |  |
| rhoI | 850.40  | kg/m3 | 308.15 | Measurement and correlation of density and viscosity of n-hexadecane with three fatty acid ethyl esters      |  |
| rhoI | 846.50  | kg/m3 | 313.15 | Measurement and correlation of density and viscosity of n-hexadecane with three fatty acid ethyl esters      |  |
| rhoI | 842.60  | kg/m3 | 318.15 | Measurement and correlation of density and viscosity of n-hexadecane with three fatty acid ethyl esters      |  |
| rhoI | 838.70  | kg/m3 | 323.15 | Measurement and correlation of density and viscosity of n-hexadecane with three fatty acid ethyl esters      |  |
| rhoI | 862.16  | kg/m3 | 293.15 | Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane |  |
| rhoI | 858.25  | kg/m3 | 298.15 | Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane |  |

|        |        |       |        |                                                                                                              |
|--------|--------|-------|--------|--------------------------------------------------------------------------------------------------------------|
| rhoI   | 854.36 | kg/m3 | 303.15 | Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane |
| rhoI   | 850.46 | kg/m3 | 308.15 | Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane |
| rhoI   | 846.56 | kg/m3 | 313.15 | Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane |
| rhoI   | 842.66 | kg/m3 | 318.15 | Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane |
| rhoI   | 838.75 | kg/m3 | 323.15 | Density, Viscosity, and Refractive Index of Binary Mixtures of Fatty Acid Ethyl Esters with Ethylcyclohexane |
| tcondI | 0.15   | W/m×K | 274.73 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel    |
| tcondI | 0.15   | W/m×K | 284.69 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel    |

|        |      |       |        |                                                                                                           |  |
|--------|------|-------|--------|-----------------------------------------------------------------------------------------------------------|--|
| tcondl | 0.15 | W/m×K | 294.56 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |  |
| tcondl | 0.14 | W/m×K | 304.59 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |  |
| tcondl | 0.14 | W/m×K | 314.47 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |  |
| tcondl | 0.14 | W/m×K | 324.41 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |  |
| tcondl | 0.14 | W/m×K | 334.28 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |  |
| tcondl | 0.14 | W/m×K | 344.09 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |  |
| tcondl | 0.13 | W/m×K | 349.21 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |  |

|        |      |       |        |                                                                                                           |
|--------|------|-------|--------|-----------------------------------------------------------------------------------------------------------|
| tcondl | 0.13 | W/m×K | 354.09 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |
| tcondl | 0.13 | W/m×K | 359.09 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |
| tcondl | 0.13 | W/m×K | 369.13 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |
| tcondl | 0.13 | W/m×K | 379.10 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |
| tcondl | 0.13 | W/m×K | 389.10 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |
| tcondl | 0.12 | W/m×K | 400.08 | Measurement on the thermal conductivity of five saturated fatty acid ethyl esters components of biodiesel |

## Correlations

| Information   | Value                         |
|---------------|-------------------------------|
| Property code | pvap                          |
| Equation      | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A      | 1.52891e+01                   |

|                             |              |
|-----------------------------|--------------|
| Coeff. B                    | -4.79892e+03 |
| Coeff. C                    | -9.24240e+01 |
| Temperature range (K), min. | 412.32       |
| Temperature range (K), max. | 573.39       |

## Datasets

### Molar heat capacity at constant pressure, J/K/mol

| Temperature, K - Liquid | Pressure, kPa - Liquid | Molar heat capacity at constant pressure, J/K/mol - Liquid |
|-------------------------|------------------------|------------------------------------------------------------|
| 313.27                  | 140.00                 | 474.00                                                     |
| 313.26                  | 5030.00                | 472.00                                                     |
| 313.26                  | 9990.00                | 471.00                                                     |
| 313.27                  | 14970.00               | 470.00                                                     |
| 313.29                  | 20040.00               | 470.00                                                     |
| 313.28                  | 25150.00               | 469.00                                                     |
| 323.22                  | 160.00                 | 480.00                                                     |
| 323.23                  | 4980.00                | 478.00                                                     |
| 323.23                  | 10110.00               | 477.00                                                     |
| 323.23                  | 14920.00               | 476.00                                                     |
| 323.22                  | 20140.00               | 475.00                                                     |
| 323.22                  | 25150.00               | 474.00                                                     |
| 333.20                  | 140.00                 | 487.00                                                     |
| 333.20                  | 4920.00                | 485.00                                                     |
| 333.20                  | 10150.00               | 483.00                                                     |
| 333.20                  | 15060.00               | 482.00                                                     |
| 333.20                  | 19970.00               | 481.00                                                     |
| 333.21                  | 25020.00               | 480.00                                                     |
| 343.15                  | 140.00                 | 493.00                                                     |
| 343.16                  | 5160.00                | 491.00                                                     |
| 343.16                  | 10270.00               | 489.00                                                     |
| 343.19                  | 15130.00               | 488.00                                                     |
| 343.19                  | 20220.00               | 487.00                                                     |
| 343.21                  | 25180.00               | 486.00                                                     |
| 353.14                  | 180.00                 | 501.00                                                     |
| 353.14                  | 4970.00                | 498.00                                                     |
| 353.17                  | 9950.00                | 496.00                                                     |
| 353.17                  | 14920.00               | 494.00                                                     |

|        |          |        |
|--------|----------|--------|
| 353.17 | 20020.00 | 492.00 |
| 353.18 | 24950.00 | 491.00 |
| 363.17 | 110.00   | 508.00 |
| 363.18 | 5010.00  | 507.00 |
| 363.29 | 10190.00 | 505.00 |
| 363.29 | 15070.00 | 503.00 |
| 363.29 | 20150.00 | 501.00 |
| 363.29 | 25100.00 | 500.00 |
| 373.19 | 110.00   | 516.00 |
| 373.20 | 4900.00  | 514.00 |
| 373.21 | 10170.00 | 512.00 |
| 373.21 | 15020.00 | 511.00 |
| 373.22 | 19850.00 | 509.00 |
| 373.25 | 24930.00 | 508.00 |
| 383.23 | 100.00   | 523.00 |
| 383.23 | 5000.00  | 521.00 |
| 383.23 | 10040.00 | 520.00 |
| 383.24 | 15080.00 | 518.00 |
| 383.25 | 19940.00 | 517.00 |
| 383.28 | 25150.00 | 515.00 |
| 393.22 | 110.00   | 532.00 |
| 393.20 | 4910.00  | 530.00 |
| 393.22 | 10100.00 | 530.00 |
| 393.27 | 15020.00 | 529.00 |
| 393.23 | 19780.00 | 528.00 |
| 393.27 | 24830.00 | 527.00 |

Reference

<https://www.doi.org/10.1016/j.fluid.2018.09.017>

## Mass density, kg/m3

| Pressure, kPa - Liquid | Temperature, K - Liquid | Mass density, kg/m3 - Liquid |
|------------------------|-------------------------|------------------------------|
| 100.00                 | 283.15                  | 869.69                       |
| 1000.00                | 283.15                  | 870.36                       |
| 3000.00                | 283.15                  | 871.92                       |
| 5000.00                | 283.15                  | 872.91                       |
| 10000.00               | 283.15                  | 876.08                       |
| 15000.00               | 283.15                  | 878.96                       |
| 20000.00               | 283.15                  | 881.89                       |
| 25000.00               | 283.15                  | 884.58                       |
| 30000.00               | 283.15                  | 887.29                       |

|          |        |        |
|----------|--------|--------|
| 35000.00 | 283.15 | 890.05 |
| 40000.00 | 283.15 | 892.47 |
| 50000.00 | 283.15 | 897.22 |
| 60000.00 | 283.15 | 901.93 |
| 100.00   | 293.15 | 862.5  |
| 1000.00  | 293.15 | 863.0  |
| 3000.00  | 293.15 | 864.24 |
| 5000.00  | 293.15 | 865.2  |
| 10000.00 | 293.15 | 868.58 |
| 15000.00 | 293.15 | 871.64 |
| 20000.00 | 293.15 | 874.58 |
| 25000.00 | 293.15 | 877.55 |
| 30000.00 | 293.15 | 880.26 |
| 35000.00 | 293.15 | 882.89 |
| 40000.00 | 293.15 | 885.52 |
| 50000.00 | 293.15 | 890.85 |
| 60000.00 | 293.15 | 895.29 |
| 100.00   | 303.15 | 854.28 |
| 1000.00  | 303.15 | 855.02 |
| 3000.00  | 303.15 | 856.39 |
| 5000.00  | 303.15 | 857.69 |
| 10000.00 | 303.15 | 860.98 |
| 15000.00 | 303.15 | 864.33 |
| 20000.00 | 303.15 | 867.23 |
| 25000.00 | 303.15 | 870.25 |
| 30000.00 | 303.15 | 873.21 |
| 35000.00 | 303.15 | 876.08 |
| 40000.00 | 303.15 | 878.71 |
| 50000.00 | 303.15 | 883.88 |
| 60000.00 | 303.15 | 888.85 |
| 100.00   | 313.15 | 846.91 |
| 1000.00  | 313.15 | 847.32 |
| 3000.00  | 313.15 | 848.68 |
| 5000.00  | 313.15 | 850.07 |
| 10000.00 | 313.15 | 853.51 |
| 15000.00 | 313.15 | 856.86 |
| 20000.00 | 313.15 | 860.1  |
| 25000.00 | 313.15 | 863.29 |
| 30000.00 | 313.15 | 866.24 |
| 35000.00 | 313.15 | 869.1  |
| 40000.00 | 313.15 | 871.83 |
| 50000.00 | 313.15 | 877.43 |
| 60000.00 | 313.15 | 882.35 |
| 100.00   | 323.15 | 838.9  |

|          |        |        |
|----------|--------|--------|
| 1000.00  | 323.15 | 839.64 |
| 3000.00  | 323.15 | 841.1  |
| 5000.00  | 323.15 | 842.59 |
| 10000.00 | 323.15 | 846.29 |
| 15000.00 | 323.15 | 849.77 |
| 20000.00 | 323.15 | 853.3  |
| 25000.00 | 323.15 | 856.35 |
| 30000.00 | 323.15 | 859.5  |
| 35000.00 | 323.15 | 862.45 |
| 40000.00 | 323.15 | 865.48 |
| 50000.00 | 323.15 | 871.16 |
| 60000.00 | 323.15 | 876.11 |
| 100.00   | 333.15 | 831.05 |
| 1000.00  | 333.15 | 831.72 |
| 3000.00  | 333.15 | 833.53 |
| 5000.00  | 333.15 | 835.15 |
| 10000.00 | 333.15 | 838.84 |
| 15000.00 | 333.15 | 842.47 |
| 20000.00 | 333.15 | 846.07 |
| 25000.00 | 333.15 | 849.47 |
| 30000.00 | 333.15 | 852.73 |
| 35000.00 | 333.15 | 855.75 |
| 40000.00 | 333.15 | 859.06 |
| 50000.00 | 333.15 | 864.9  |
| 60000.00 | 333.15 | 870.44 |
| 100.00   | 343.15 | 823.11 |
| 1000.00  | 343.15 | 824.13 |
| 3000.00  | 343.15 | 825.84 |
| 5000.00  | 343.15 | 827.55 |
| 10000.00 | 343.15 | 831.53 |
| 15000.00 | 343.15 | 835.33 |
| 20000.00 | 343.15 | 839.18 |
| 25000.00 | 343.15 | 842.57 |
| 30000.00 | 343.15 | 846.08 |
| 35000.00 | 343.15 | 849.44 |
| 40000.00 | 343.15 | 852.46 |
| 50000.00 | 343.15 | 858.61 |
| 60000.00 | 343.15 | 864.08 |
| 100.00   | 353.15 | 815.47 |
| 1000.00  | 353.15 | 816.33 |
| 3000.00  | 353.15 | 818.26 |
| 5000.00  | 353.15 | 819.99 |
| 10000.00 | 353.15 | 824.24 |
| 15000.00 | 353.15 | 828.35 |

|          |        |        |
|----------|--------|--------|
| 20000.00 | 353.15 | 832.01 |
| 25000.00 | 353.15 | 835.81 |
| 30000.00 | 353.15 | 839.36 |
| 35000.00 | 353.15 | 842.72 |
| 40000.00 | 353.15 | 846.01 |
| 50000.00 | 353.15 | 852.29 |
| 60000.00 | 353.15 | 858.27 |
| 100.00   | 363.15 | 807.52 |
| 1000.00  | 363.15 | 808.53 |
| 3000.00  | 363.15 | 810.45 |
| 5000.00  | 363.15 | 812.32 |
| 10000.00 | 363.15 | 816.46 |
| 15000.00 | 363.15 | 821.01 |
| 20000.00 | 363.15 | 824.82 |
| 25000.00 | 363.15 | 828.56 |
| 30000.00 | 363.15 | 832.36 |
| 35000.00 | 363.15 | 835.98 |
| 40000.00 | 363.15 | 839.55 |
| 50000.00 | 363.15 | 845.99 |
| 60000.00 | 363.15 | 852.14 |

Reference

<https://www.doi.org/10.1016/j.jct.2016.08.027>

| Temperature, K | Pressure, kPa | Mass density, kg/m3 |
|----------------|---------------|---------------------|
| 303.06         | 100.00        | 853.9               |
| 303.07         | 3050.00       | 856.6               |
| 303.26         | 5990.00       | 858.4               |
| 303.22         | 9020.00       | 860.5               |
| 303.23         | 11990.00      | 862.5               |
| 303.24         | 15030.00      | 864.5               |
| 313.08         | 100.00        | 846.3               |
| 313.08         | 3010.00       | 848.3               |
| 313.10         | 5980.00       | 850.4               |
| 313.15         | 9030.00       | 852.6               |
| 313.17         | 12010.00      | 854.4               |
| 313.26         | 15030.00      | 857.5               |
| 323.14         | 100.00        | 838.3               |
| 323.09         | 3050.00       | 840.8               |
| 323.17         | 5980.00       | 842.9               |
| 323.17         | 8980.00       | 845.0               |
| 323.17         | 11990.00      | 847.0               |
| 323.18         | 15020.00      | 849.0               |
| 333.17         | 100.00        | 830.8               |

|        |          |       |
|--------|----------|-------|
| 333.17 | 3010.00  | 833.0 |
| 333.07 | 6000.00  | 835.8 |
| 333.20 | 9040.00  | 838.1 |
| 333.17 | 12040.00 | 840.3 |
| 333.15 | 15040.00 | 842.5 |
| 342.95 | 100.00   | 823.2 |
| 343.00 | 3000.00  | 825.3 |
| 343.19 | 5980.00  | 828.3 |
| 343.28 | 9020.00  | 830.8 |
| 343.19 | 11980.00 | 832.8 |
| 343.19 | 15020.00 | 834.9 |
| 353.15 | 100.00   | 815.3 |
| 353.15 | 3050.00  | 818.4 |
| 353.20 | 6030.00  | 820.9 |
| 353.19 | 9020.00  | 823.2 |
| 353.18 | 12010.00 | 825.6 |
| 353.19 | 15020.00 | 827.9 |

Reference

<https://www.doi.org/10.1016/j.tca.2018.03.007>

## Speed of sound, m/s

| Temperature, K - Liquid | Pressure, kPa - Liquid | Speed of sound, m/s - Liquid |
|-------------------------|------------------------|------------------------------|
| 293.15                  | 100.00                 | 1339.9                       |
| 293.15                  | 10000.00               | 1390.8                       |
| 293.15                  | 20000.00               | 1436.7                       |
| 293.15                  | 30000.00               | 1479.3                       |
| 293.15                  | 40000.00               | 1519.0                       |
| 293.15                  | 50000.00               | 1555.9                       |
| 293.15                  | 60000.00               | 1591.9                       |
| 293.15                  | 70000.00               | 1626.2                       |
| 293.15                  | 80000.00               | 1659.7                       |
| 293.15                  | 90000.00               | 1690.9                       |
| 293.15                  | 100000.00              | 1720.9                       |
| 293.15                  | 120000.00              | 1778.5                       |
| 313.15                  | 100.00                 | 1266.1                       |
| 313.15                  | 10000.00               | 1317.6                       |
| 313.15                  | 20000.00               | 1365.0                       |
| 313.15                  | 30000.00               | 1409.3                       |
| 313.15                  | 40000.00               | 1452.1                       |
| 313.15                  | 50000.00               | 1491.4                       |

|        |           |        |
|--------|-----------|--------|
| 313.15 | 60000.00  | 1529.2 |
| 313.15 | 70000.00  | 1564.8 |
| 313.15 | 80000.00  | 1600.2 |
| 313.15 | 90000.00  | 1632.3 |
| 313.15 | 100000.00 | 1663.0 |
| 313.15 | 120000.00 | 1721.9 |
| 313.15 | 140000.00 | 1777.9 |
| 313.15 | 160000.00 | 1830.9 |
| 333.15 | 100.00    | 1194.0 |
| 333.15 | 10000.00  | 1250.3 |
| 333.15 | 20000.00  | 1300.9 |
| 333.15 | 30000.00  | 1348.0 |
| 333.15 | 40000.00  | 1393.4 |
| 333.15 | 50000.00  | 1434.3 |
| 333.15 | 60000.00  | 1473.3 |
| 333.15 | 70000.00  | 1509.8 |
| 333.15 | 80000.00  | 1545.4 |
| 333.15 | 90000.00  | 1578.6 |
| 333.15 | 100000.00 | 1610.9 |
| 333.15 | 120000.00 | 1674.1 |
| 333.15 | 140000.00 | 1730.4 |
| 333.15 | 160000.00 | 1782.7 |
| 333.15 | 180000.00 | 1835.3 |
| 333.15 | 200000.00 | 1883.8 |
| 353.15 | 100.00    | 1125.7 |
| 353.15 | 10000.00  | 1186.0 |
| 353.15 | 20000.00  | 1240.6 |
| 353.15 | 30000.00  | 1290.3 |
| 353.15 | 40000.00  | 1337.1 |
| 353.15 | 50000.00  | 1379.7 |
| 353.15 | 60000.00  | 1419.8 |
| 353.15 | 70000.00  | 1458.8 |
| 353.15 | 80000.00  | 1496.2 |
| 353.15 | 90000.00  | 1530.6 |
| 353.15 | 100000.00 | 1564.4 |
| 353.15 | 120000.00 | 1627.0 |
| 353.15 | 140000.00 | 1685.1 |
| 353.15 | 160000.00 | 1740.7 |
| 353.15 | 180000.00 | 1793.6 |
| 353.15 | 200000.00 | 1843.5 |

Reference

<https://www.doi.org/10.1016/j.jct.2017.12.020>

# Sources

|                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
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| Experimental Vapor Pressures of Five Saturated Fatty Acid Ethyl Ester (FAEE)                                                                                                                                                                                                                                                        | <a href="https://www.doi.org/10.1021/je200730m">https://www.doi.org/10.1021/je200730m</a>                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
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| Crippen Method:                                                                                                                                                                                                                                                                                                                     | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
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## Legend

|        |                                                 |
|--------|-------------------------------------------------|
| chl:   | Standard liquid enthalpy of combustion          |
| 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    |
| hfus:  | Enthalpy of fusion at standard conditions       |
| hfust: | Enthalpy of fusion at a given temperature       |
| hvap:  | 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>rho:</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>tcondl:</b>  | Liquid thermal conductivity                     |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>tt:</b>      | Triple Point Temperature                        |
| <b>vc:</b>      | Critical Volume                                 |

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