

# Nonanoic acid, ethyl ester

|                      |                                                                                           |
|----------------------|-------------------------------------------------------------------------------------------|
| Other names:         | Ethyl n-nonanoate<br>Ethyl nonanoate<br>Ethyl nonylate<br>Ethyl pelargonate<br>Wine ether |
| Inchi:               | InChI=1S/C11H22O2/c1-3-5-6-7-8-9-10-11(12)13-4-2/h3-10H2,1-2H3                            |
| InchiKey:            | BYEVBITUADOIGY-UHFFFAOYSA-N                                                               |
| Formula:             | C11H22O2                                                                                  |
| SMILES:              | CCCCCCCCC(=O)OCC                                                                          |
| Mol. weight [g/mol]: | 186.29                                                                                    |
| CAS:                 | 123-29-5                                                                                  |

## Physical Properties

| Property code | Value          | Unit   | Source                               |
|---------------|----------------|--------|--------------------------------------|
| gf            | -192.18        | kJ/mol | Joback Method                        |
| hf            | -590.00 ± 3.00 | kJ/mol | NIST Webbook                         |
| hfl           | -653.90 ± 2.10 | kJ/mol | NIST Webbook                         |
| hfus          | 27.03          | kJ/mol | Joback Method                        |
| hvap          | 63.90          | kJ/mol | NIST Webbook                         |
| hvap          | 64.00 ± 1.00   | kJ/mol | NIST Webbook                         |
| log10ws       | -3.80          |        | Estimated Solubility Method          |
| log10ws       | -3.80          |        | Aqueous Solubility Prediction Method |
| logp          | 3.300          |        | Crippen Method                       |
| mcvol         | 173.290        | ml/mol | McGowan Method                       |
| pc            | 2014.51        | kPa    | Joback Method                        |
| rinpol        | 1280.00        |        | NIST Webbook                         |
| rinpol        | 1295.00        |        | NIST Webbook                         |
| rinpol        | 1280.00        |        | NIST Webbook                         |
| rinpol        | 1279.00        |        | NIST Webbook                         |
| rinpol        | 1279.00        |        | NIST Webbook                         |
| rinpol        | 1277.00        |        | NIST Webbook                         |
| rinpol        | 1281.00        |        | NIST Webbook                         |
| rinpol        | 1268.00        |        | NIST Webbook                         |
| rinpol        | 1319.00        |        | NIST Webbook                         |
| rinpol        | 1294.00        |        | NIST Webbook                         |

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| rinpol | 1296.00 | NIST Webbook |
| rinpol | 1294.00 | NIST Webbook |
| rinpol | 1293.00 | NIST Webbook |
| rinpol | 1296.00 | NIST Webbook |
| rinpol | 1300.00 | NIST Webbook |
| rinpol | 1298.00 | NIST Webbook |
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| rinpol | 1280.00 | NIST Webbook |
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| rinpol | 1281.00 | NIST Webbook |
| rinpol | 1279.00 | NIST Webbook |
| rinpol | 1319.00 | NIST Webbook |

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|--------|---------|--------------|
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| rinpol | 1284.00 | NIST Webbook |
| rinpol | 1284.00 | NIST Webbook |
| rinpol | 1304.00 | NIST Webbook |
| rinpol | 1298.00 | NIST Webbook |
| ripol  | 1568.00 | NIST Webbook |
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| ripol  | 1535.00 | NIST Webbook |

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|-------|---------------|---------|--------------------------------------|
| ripol | 1553.00       |         | NIST Webbook                         |
| ripol | 1526.00       |         | NIST Webbook                         |
| ripol | 1528.00       |         | NIST Webbook                         |
| ripol | 1537.00       |         | NIST Webbook                         |
| ripol | 1528.00       |         | NIST Webbook                         |
| ripol | 1563.00       |         | NIST Webbook                         |
| ripol | 1530.00       |         | NIST Webbook                         |
| ripol | 1531.00       |         | NIST Webbook                         |
| ripol | 1521.00       |         | NIST Webbook                         |
| ripol | 1570.00       |         | NIST Webbook                         |
| ripol | 1530.00       |         | NIST Webbook                         |
| tb    | 500.15 ± 1.00 | K       | NIST Webbook                         |
| tb    | 500.15 ± 1.00 | K       | NIST Webbook                         |
| tb    | 490.15 ± 8.00 | K       | NIST Webbook                         |
| tb    | 500.15 ± 2.00 | K       | NIST Webbook                         |
| tc    | 663.90 ± 3.00 | K       | NIST Webbook                         |
| tc    | 673.96 ± 6.00 | K       | NIST Webbook                         |
| tf    | 232.80        | K       | Aqueous Solubility Prediction Method |
| tf    | 228.70 ± 0.20 | K       | NIST Webbook                         |
| vc    | 0.675         | m3/kmol | Joback Method                        |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 496.57    | J/mol×K | 698.36          | Joback Method |
| cpg           | 415.24    | J/mol×K | 527.37          | Joback Method |
| cpg           | 430.19    | J/mol×K | 555.87          | Joback Method |
| cpg           | 444.58    | J/mol×K | 584.37          | Joback Method |
| cpg           | 458.41    | J/mol×K | 612.87          | Joback Method |
| cpg           | 471.67    | J/mol×K | 641.36          | Joback Method |
| cpg           | 484.39    | J/mol×K | 669.86          | Joback Method |
| dvisc         | 0.0002056 | Pa×s    | 527.37          | Joback Method |
| dvisc         | 0.0032030 | Pa×s    | 285.89          | Joback Method |
| dvisc         | 0.0015281 | Pa×s    | 326.14          | Joback Method |
| dvisc         | 0.0008577 | Pa×s    | 366.38          | Joback Method |
| dvisc         | 0.0005398 | Pa×s    | 406.63          | Joback Method |
| dvisc         | 0.0003692 | Pa×s    | 446.88          | Joback Method |
| dvisc         | 0.0002689 | Pa×s    | 487.12          | Joback Method |

|      |        |       |        |                                                                                                                                                                                   |
|------|--------|-------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| rhoI | 866.30 | kg/m3 | 293.20 | Modeling extraction equilibria of butyric acid distributed between water and tri-n-butyl amine/diluent or tri-n-butyl phosphate/diluent system:<br>Extension of the LSER approach |
|------|--------|-------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 392.20 | K    | 3.10           | NIST Webbook |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.56251e+01                   |
| Coeff. B                    | -4.55414e+03                  |
| Coeff. C                    | -8.01920e+01                  |
| Temperature range (K), min. | 377.12                        |
| Temperature range (K), max. | 521.76                        |

## 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 |
|-------------------------|------------------------|------------------------------------------------------------|
| 303.31                  | 110.00                 | 371.00                                                     |

|        |          |        |
|--------|----------|--------|
| 303.25 | 5000.00  | 371.00 |
| 303.22 | 9980.00  | 370.00 |
| 303.21 | 15150.00 | 369.00 |
| 303.24 | 20090.00 | 369.00 |
| 303.27 | 24930.00 | 368.00 |
| 313.23 | 170.00   | 377.00 |
| 313.26 | 5090.00  | 377.00 |
| 313.24 | 9850.00  | 376.00 |
| 313.22 | 14910.00 | 376.00 |
| 313.21 | 19900.00 | 375.00 |
| 313.24 | 24930.00 | 374.00 |
| 323.22 | 110.00   | 386.00 |
| 323.19 | 4970.00  | 385.00 |
| 323.23 | 10020.00 | 384.00 |
| 323.26 | 15190.00 | 383.00 |
| 323.24 | 20090.00 | 382.00 |
| 323.22 | 24920.00 | 382.00 |
| 333.18 | 140.00   | 394.00 |
| 333.16 | 4930.00  | 393.00 |
| 333.18 | 9950.00  | 393.00 |
| 333.21 | 15110.00 | 393.00 |
| 333.19 | 20150.00 | 392.00 |
| 333.23 | 25020.00 | 392.00 |
| 343.20 | 110.00   | 401.00 |
| 343.19 | 5070.00  | 400.00 |
| 343.19 | 9940.00  | 400.00 |
| 343.19 | 14950.00 | 400.00 |
| 343.21 | 19870.00 | 399.00 |
| 343.22 | 25210.00 | 399.00 |
| 353.14 | 160.00   | 407.00 |
| 353.11 | 4910.00  | 407.00 |
| 353.14 | 10160.00 | 406.00 |
| 353.15 | 14930.00 | 406.00 |
| 353.20 | 20210.00 | 405.00 |
| 353.23 | 25190.00 | 405.00 |
| 363.12 | 110.00   | 414.00 |
| 363.14 | 5090.00  | 413.00 |
| 363.17 | 10020.00 | 413.00 |
| 363.16 | 15060.00 | 412.00 |
| 363.17 | 20130.00 | 411.00 |
| 363.19 | 25160.00 | 410.00 |
| 373.12 | 100.00   | 420.00 |
| 373.12 | 4830.00  | 420.00 |
| 373.13 | 10020.00 | 419.00 |

|        |          |        |
|--------|----------|--------|
| 373.13 | 15150.00 | 418.00 |
| 373.14 | 20170.00 | 418.00 |
| 373.14 | 24950.00 | 417.00 |
| 383.18 | 160.00   | 427.00 |
| 383.20 | 4950.00  | 426.00 |
| 383.20 | 10190.00 | 425.00 |
| 383.20 | 15000.00 | 425.00 |
| 383.22 | 20130.00 | 424.00 |
| 383.22 | 24950.00 | 424.00 |
| 393.18 | 110.00   | 434.00 |
| 393.18 | 5090.00  | 433.00 |
| 393.18 | 10020.00 | 433.00 |
| 393.19 | 15150.00 | 433.00 |
| 393.20 | 20190.00 | 432.00 |
| 393.24 | 24960.00 | 432.00 |

Reference

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

## Speed of sound, m/s

| Temperature, K - Liquid | Pressure, kPa - Liquid | Speed of sound, m/s - Liquid |
|-------------------------|------------------------|------------------------------|
| 295.67                  | 100.00                 | 1303.3                       |
| 303.48                  | 100.00                 | 1273.9                       |
| 313.77                  | 100.00                 | 1224.9                       |
| 323.68                  | 100.00                 | 1183.3                       |
| 334.94                  | 100.00                 | 1142.9                       |
| 343.51                  | 100.00                 | 1107.8                       |
| 354.18                  | 100.00                 | 1065.4                       |
| 364.18                  | 100.00                 | 1028.8                       |
| 371.99                  | 100.00                 | 1003.0                       |
| 381.89                  | 100.00                 | 965.2                        |
| 391.89                  | 100.00                 | 932.1                        |
| 405.01                  | 100.00                 | 884.0                        |
| 413.84                  | 100.00                 | 861.2                        |
| 422.07                  | 100.00                 | 827.6                        |
| 432.93                  | 100.00                 | 797.1                        |
| 443.70                  | 100.00                 | 767.3                        |
| 452.83                  | 100.00                 | 739.6                        |
| 464.19                  | 100.00                 | 703.5                        |
| 471.88                  | 100.00                 | 683.0                        |
| 482.75                  | 100.00                 | 652.6                        |

|        |         |        |
|--------|---------|--------|
| 295.53 | 1000.00 | 1318.3 |
| 303.26 | 1000.00 | 1278.4 |
| 313.14 | 1000.00 | 1242.7 |
| 324.85 | 1000.00 | 1195.5 |
| 333.21 | 1000.00 | 1163.1 |
| 343.24 | 1000.00 | 1123.8 |
| 352.22 | 1000.00 | 1085.5 |
| 363.30 | 1000.00 | 1046.0 |
| 371.91 | 1000.00 | 1012.3 |
| 384.30 | 1000.00 | 971.3  |
| 391.75 | 1000.00 | 939.5  |
| 403.31 | 1000.00 | 902.3  |
| 412.98 | 1000.00 | 870.1  |
| 421.83 | 1000.00 | 842.1  |
| 431.53 | 1000.00 | 808.9  |
| 442.94 | 1000.00 | 779.7  |
| 452.50 | 1000.00 | 750.6  |
| 462.68 | 1000.00 | 720.1  |
| 471.87 | 1000.00 | 693.4  |
| 482.55 | 1000.00 | 665.4  |
| 493.00 | 1000.00 | 637.4  |
| 502.95 | 1000.00 | 607.9  |
| 513.20 | 1000.00 | 581.3  |
| 522.13 | 1000.00 | 555.5  |
| 533.35 | 1000.00 | 519.4  |
| 543.62 | 1000.00 | 491.0  |
| 552.71 | 1000.00 | 458.7  |
| 562.08 | 1000.00 | 428.6  |
| 571.96 | 1000.00 | 387.2  |
| 295.41 | 3000.00 | 1327.1 |
| 303.22 | 3000.00 | 1296.2 |
| 313.56 | 3000.00 | 1252.4 |
| 324.78 | 3000.00 | 1204.3 |
| 332.93 | 3000.00 | 1175.1 |
| 342.88 | 3000.00 | 1137.2 |
| 351.94 | 3000.00 | 1098.9 |
| 362.97 | 3000.00 | 1063.9 |
| 372.73 | 3000.00 | 1024.3 |
| 381.96 | 3000.00 | 995.2  |
| 391.81 | 3000.00 | 961.1  |
| 403.46 | 3000.00 | 921.8  |
| 412.73 | 3000.00 | 893.7  |
| 422.02 | 3000.00 | 862.5  |
| 432.05 | 3000.00 | 827.6  |

|        |         |        |
|--------|---------|--------|
| 443.11 | 3000.00 | 796.4  |
| 452.88 | 3000.00 | 771.1  |
| 462.31 | 3000.00 | 743.5  |
| 471.80 | 3000.00 | 718.5  |
| 482.56 | 3000.00 | 691.9  |
| 492.57 | 3000.00 | 660.7  |
| 502.65 | 3000.00 | 635.1  |
| 512.83 | 3000.00 | 609.6  |
| 522.31 | 3000.00 | 583.9  |
| 533.60 | 3000.00 | 552.1  |
| 542.72 | 3000.00 | 528.8  |
| 552.52 | 3000.00 | 500.5  |
| 562.48 | 3000.00 | 468.4  |
| 571.78 | 3000.00 | 435.9  |
| 582.39 | 3000.00 | 393.3  |
| 591.81 | 3000.00 | 351.2  |
| 295.35 | 5000.00 | 1336.6 |
| 303.41 | 5000.00 | 1298.0 |
| 314.03 | 5000.00 | 1262.6 |
| 323.64 | 5000.00 | 1215.5 |
| 334.21 | 5000.00 | 1185.0 |
| 343.12 | 5000.00 | 1153.6 |
| 353.27 | 5000.00 | 1106.1 |
| 361.97 | 5000.00 | 1078.7 |
| 371.77 | 5000.00 | 1046.8 |
| 381.51 | 5000.00 | 1011.2 |
| 391.70 | 5000.00 | 974.2  |
| 403.82 | 5000.00 | 929.8  |
| 413.05 | 5000.00 | 904.2  |
| 421.50 | 5000.00 | 875.4  |
| 431.84 | 5000.00 | 850.9  |
| 443.15 | 5000.00 | 814.1  |
| 452.65 | 5000.00 | 786.9  |
| 462.49 | 5000.00 | 763.0  |
| 471.86 | 5000.00 | 737.7  |
| 482.62 | 5000.00 | 709.2  |
| 492.67 | 5000.00 | 681.7  |
| 503.42 | 5000.00 | 655.5  |
| 512.90 | 5000.00 | 633.5  |
| 522.36 | 5000.00 | 609.3  |
| 533.69 | 5000.00 | 581.4  |
| 542.91 | 5000.00 | 553.5  |
| 552.72 | 5000.00 | 527.6  |
| 562.32 | 5000.00 | 499.9  |

|        |          |        |
|--------|----------|--------|
| 572.37 | 5000.00  | 472.0  |
| 582.01 | 5000.00  | 439.9  |
| 592.38 | 5000.00  | 398.5  |
| 295.29 | 7000.00  | 1342.4 |
| 303.30 | 7000.00  | 1307.0 |
| 313.45 | 7000.00  | 1266.0 |
| 322.95 | 7000.00  | 1231.4 |
| 334.21 | 7000.00  | 1191.7 |
| 343.31 | 7000.00  | 1157.3 |
| 353.32 | 7000.00  | 1114.4 |
| 362.59 | 7000.00  | 1085.6 |
| 373.26 | 7000.00  | 1045.8 |
| 383.69 | 7000.00  | 1011.5 |
| 391.74 | 7000.00  | 985.8  |
| 403.36 | 7000.00  | 943.9  |
| 412.81 | 7000.00  | 917.8  |
| 422.00 | 7000.00  | 891.0  |
| 431.88 | 7000.00  | 861.7  |
| 443.00 | 7000.00  | 835.6  |
| 452.64 | 7000.00  | 805.0  |
| 462.34 | 7000.00  | 783.1  |
| 471.86 | 7000.00  | 756.6  |
| 482.58 | 7000.00  | 727.2  |
| 492.66 | 7000.00  | 704.9  |
| 502.91 | 7000.00  | 681.8  |
| 512.78 | 7000.00  | 655.0  |
| 522.19 | 7000.00  | 631.9  |
| 533.43 | 7000.00  | 605.6  |
| 542.79 | 7000.00  | 583.0  |
| 552.61 | 7000.00  | 558.1  |
| 562.40 | 7000.00  | 532.0  |
| 572.13 | 7000.00  | 504.6  |
| 582.26 | 7000.00  | 473.6  |
| 592.79 | 7000.00  | 438.3  |
| 295.24 | 10000.00 | 1348.5 |
| 303.18 | 10000.00 | 1318.0 |
| 313.08 | 10000.00 | 1283.3 |
| 323.39 | 10000.00 | 1246.8 |
| 332.89 | 10000.00 | 1208.8 |
| 343.10 | 10000.00 | 1170.1 |
| 352.39 | 10000.00 | 1135.0 |
| 363.00 | 10000.00 | 1106.9 |
| 373.24 | 10000.00 | 1068.4 |
| 383.17 | 10000.00 | 1037.3 |

|        |          |        |
|--------|----------|--------|
| 391.74 | 10000.00 | 1009.8 |
| 403.47 | 10000.00 | 968.6  |
| 412.73 | 10000.00 | 936.6  |
| 421.98 | 10000.00 | 916.0  |
| 431.86 | 10000.00 | 888.7  |
| 443.02 | 10000.00 | 860.3  |
| 452.68 | 10000.00 | 835.1  |
| 462.43 | 10000.00 | 804.8  |
| 471.95 | 10000.00 | 783.4  |
| 482.62 | 10000.00 | 759.9  |
| 492.48 | 10000.00 | 735.7  |
| 503.08 | 10000.00 | 709.9  |
| 512.80 | 10000.00 | 689.4  |
| 522.38 | 10000.00 | 662.0  |
| 533.52 | 10000.00 | 637.0  |
| 542.76 | 10000.00 | 619.6  |
| 552.76 | 10000.00 | 596.5  |
| 562.45 | 10000.00 | 574.7  |
| 572.32 | 10000.00 | 549.0  |
| 582.35 | 10000.00 | 525.5  |
| 593.15 | 10000.00 | 495.3  |

Reference

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## Sources

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Speed of Sound and Derived Properties of Ethyl Nonanoate: Liquid Phase Equilibria for Mixtures of (Water + Morpholine + Ethyl Nonanoate, Dimethyl Phthalate, or Isoamyl Alcohol) at 298.15 K:

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# Legend

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                                   |
| <b>cpl:</b>     | Liquid phase 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>hfl:</b>     | Liquid phase 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>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>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>tbrp:</b>    | Boiling point at reduced pressure                         |
| <b>tc:</b>      | Critical Temperature                                      |
| <b>tf:</b>      | Normal melting (fusion) point                             |
| <b>vc:</b>      | Critical Volume                                           |

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