

# 3-Pentanol, 3-methyl-

|                      |                                                                                                                                                                                                                              |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-ethyl-2-butanol<br>3-Methyl-3-pentanol<br>3-Methyl-pentanol-(3)<br>3-Methylpentan-3-ol<br>3-hydroxy-3-methylpentane<br>3-methyl-3-pentyl alcohol<br>Methyl-3 pentanol-3<br>Methyldiaethylcarbinol<br>Methyldiethylcarbinol |
| Inchi:               | InChI=1S/C6H14O/c1-4-6(3,7)5-2/h7H,4-5H2,1-3H3                                                                                                                                                                               |
| InchiKey:            | FRDAATYAJDYRNW-UHFFFAOYSA-N                                                                                                                                                                                                  |
| Formula:             | C6H14O                                                                                                                                                                                                                       |
| SMILES:              | CCC(C)(O)CC                                                                                                                                                                                                                  |
| Mol. weight [g/mol]: | 102.17                                                                                                                                                                                                                       |
| CAS:                 | 77-74-7                                                                                                                                                                                                                      |

## Physical Properties

| Property code | Value           | Unit   | Source                               |
|---------------|-----------------|--------|--------------------------------------|
| gf            | -134.34         | kJ/mol | Joback Method                        |
| hf            | -348.30 ± 1.20  | kJ/mol | NIST Webbook                         |
| hfl           | -404.90 ± 0.88  | kJ/mol | NIST Webbook                         |
| hfus          | 7.97            | kJ/mol | Joback Method                        |
| hvap          | 56.65 ± 0.84    | kJ/mol | NIST Webbook                         |
| hvap          | 56.70 ± 0.80    | kJ/mol | NIST Webbook                         |
| hvap          | 56.60           | kJ/mol | NIST Webbook                         |
| hvap          | 55.70 ± 0.30    | kJ/mol | NIST Webbook                         |
| log10ws       | -0.36           |        | Estimated Solubility Method          |
| log10ws       | -0.38           |        | Aqueous Solubility Prediction Method |
| logp          | 1.557           |        | Crippen Method                       |
| mcpvol        | 101.270         | ml/mol | McGowan Method                       |
| pc            | 3520.00 ± 20.00 | kPa    | NIST Webbook                         |
| pc            | 3520.00 ± 50.00 | kPa    | NIST Webbook                         |
| rinpol        | 737.00          |        | NIST Webbook                         |
| rinpol        | 733.40          |        | NIST Webbook                         |
| rinpol        | 757.00          |        | NIST Webbook                         |

|        |               |         |                                         |
|--------|---------------|---------|-----------------------------------------|
| rinpol | 757.00        |         | NIST Webbook                            |
| rinpol | 757.00        |         | NIST Webbook                            |
| rinpol | 755.90        |         | NIST Webbook                            |
| rinpol | 733.90        |         | NIST Webbook                            |
| rinpol | 749.00        |         | NIST Webbook                            |
| ripol  | 1115.00       |         | NIST Webbook                            |
| ripol  | 1119.00       |         | NIST Webbook                            |
| ripol  | 1080.00       |         | NIST Webbook                            |
| ripol  | 1080.00       |         | NIST Webbook                            |
| ripol  | 1080.00       |         | NIST Webbook                            |
| ripol  | 1108.00       |         | NIST Webbook                            |
| ripol  | 1112.00       |         | NIST Webbook                            |
| tb     | 396.05 ± 0.70 | K       | NIST Webbook                            |
| tb     | 406.65 ± 5.00 | K       | NIST Webbook                            |
| tb     | 396.15 ± 2.00 | K       | NIST Webbook                            |
| tb     | 395.85 ± 0.50 | K       | NIST Webbook                            |
| tb     | 395.15 ± 2.00 | K       | NIST Webbook                            |
| tb     | 396.15 ± 2.00 | K       | NIST Webbook                            |
| tb     | 394.00 ± 2.00 | K       | NIST Webbook                            |
| tb     | 395.65 ± 2.00 | K       | NIST Webbook                            |
| tb     | 395.40 ± 3.00 | K       | NIST Webbook                            |
| tb     | 394.55 ± 2.00 | K       | NIST Webbook                            |
| tb     | 395.15 ± 4.00 | K       | NIST Webbook                            |
| tb     | 395.55 ± 0.50 | K       | NIST Webbook                            |
| tb     | 395.65 ± 2.00 | K       | NIST Webbook                            |
| tb     | 394.05 ± 1.00 | K       | NIST Webbook                            |
| tb     | 394.65 ± 2.00 | K       | NIST Webbook                            |
| tb     | 394.40 ± 2.00 | K       | NIST Webbook                            |
| tb     | 395.15 ± 2.00 | K       | NIST Webbook                            |
| tb     | 396.20 ± 1.00 | K       | NIST Webbook                            |
| tb     | 394.15 ± 2.00 | K       | NIST Webbook                            |
| tb     | 393.40 ± 2.00 | K       | NIST Webbook                            |
| tb     | 374.65 ± 5.00 | K       | NIST Webbook                            |
| tb     | 394.15 ± 2.00 | K       | NIST Webbook                            |
| tb     | 394.15 ± 2.00 | K       | NIST Webbook                            |
| tb     | 395.60        | K       | NIST Webbook                            |
| tc     | 575.60 ± 0.80 | K       | NIST Webbook                            |
| tc     | 575.60 ± 0.60 | K       | NIST Webbook                            |
| tf     | 249.35        | K       | Aqueous Solubility<br>Prediction Method |
| tf     | 249.55 ± 0.20 | K       | NIST Webbook                            |
| vc     | 0.380         | m3/kmol | Joback Method                           |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 240.32    | J/mol×K | 511.13          | Joback Method |
| cpg           | 249.46    | J/mol×K | 539.64          | Joback Method |
| cpg           | 258.15    | J/mol×K | 568.14          | Joback Method |
| cpg           | 210.01    | J/mol×K | 425.63          | Joback Method |
| cpg           | 220.61    | J/mol×K | 454.13          | Joback Method |
| cpg           | 230.71    | J/mol×K | 482.63          | Joback Method |
| cpg           | 266.42    | J/mol×K | 596.64          | Joback Method |
| cpl           | 302.25    | J/mol×K | 298.15          | NIST Webbook  |
| cpl           | 293.38    | J/mol×K | 298.15          | NIST Webbook  |
| cpl           | 293.83    | J/mol×K | 298.15          | NIST Webbook  |
| dvisc         | 0.0002697 | Pa×s    | 425.63          | Joback Method |
| dvisc         | 0.0009643 | Pa×s    | 357.29          | Joback Method |
| dvisc         | 0.0004823 | Pa×s    | 391.46          | Joback Method |
| dvisc         | 0.1316325 | Pa×s    | 220.62          | Joback Method |
| dvisc         | 0.0234865 | Pa×s    | 254.79          | Joback Method |
| dvisc         | 0.0062994 | Pa×s    | 288.96          | Joback Method |
| dvisc         | 0.0022318 | Pa×s    | 323.12          | Joback Method |
| hvapt         | 42.10     | kJ/mol  | 345.50          | NIST Webbook  |
| hvapt         | 46.40     | kJ/mol  | 367.00          | NIST Webbook  |
| hvapt         | 40.10     | kJ/mol  | 359.50          | NIST Webbook  |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.37248e+01                   |
| Coeff. B                    | -2.62615e+03                  |
| Coeff. C                    | -1.06616e+02                  |
| Temperature range (K), min. | 302.06                        |
| Temperature range (K), max. | 418.76                        |

# Datasets

## Speed of sound, m/s

| Temperature, K - Liquid | Pressure, kPa - Liquid | Speed of sound, m/s - Liquid |
|-------------------------|------------------------|------------------------------|
| 303.15                  | 100.00                 | 1230.7                       |
| 303.15                  | 10000.00               | 1290.1                       |
| 303.15                  | 20000.00               | 1344.9                       |
| 303.15                  | 30000.00               | 1396.1                       |
| 303.15                  | 40000.00               | 1443.3                       |
| 303.15                  | 50000.00               | 1487.1                       |
| 303.15                  | 60000.00               | 1529.7                       |
| 303.15                  | 70000.00               | 1568.8                       |
| 303.15                  | 80000.00               | 1606.2                       |
| 303.15                  | 90000.00               | 1641.7                       |
| 303.15                  | 100000.00              | 1675.9                       |
| 313.15                  | 100.00                 | 1192.7                       |
| 313.15                  | 10000.00               | 1254.9                       |
| 313.15                  | 20000.00               | 1311.8                       |
| 313.15                  | 30000.00               | 1365.0                       |
| 313.15                  | 40000.00               | 1412.6                       |
| 313.15                  | 50000.00               | 1457.9                       |
| 313.15                  | 60000.00               | 1500.4                       |
| 313.15                  | 70000.00               | 1540.7                       |
| 313.15                  | 80000.00               | 1578.9                       |
| 313.15                  | 90000.00               | 1615.0                       |
| 313.15                  | 100000.00              | 1650.0                       |
| 323.15                  | 100.00                 | 1154.4                       |
| 323.15                  | 10000.00               | 1219.2                       |
| 323.15                  | 20000.00               | 1278.7                       |
| 323.15                  | 30000.00               | 1332.4                       |
| 323.15                  | 40000.00               | 1382.1                       |
| 323.15                  | 50000.00               | 1428.9                       |
| 323.15                  | 60000.00               | 1472.8                       |
| 323.15                  | 70000.00               | 1513.6                       |
| 323.15                  | 80000.00               | 1552.8                       |
| 323.15                  | 90000.00               | 1589.9                       |
| 323.15                  | 100000.00              | 1624.9                       |
| 333.15                  | 100.00                 | 1115.7                       |
| 333.15                  | 10000.00               | 1183.6                       |

|        |           |        |
|--------|-----------|--------|
| 333.15 | 20000.00  | 1245.0 |
| 333.15 | 30000.00  | 1300.4 |
| 333.15 | 40000.00  | 1351.9 |
| 333.15 | 50000.00  | 1399.7 |
| 333.15 | 60000.00  | 1444.4 |
| 333.15 | 70000.00  | 1486.1 |
| 333.15 | 80000.00  | 1525.6 |
| 333.15 | 90000.00  | 1563.8 |
| 333.15 | 100000.00 | 1599.9 |
| 343.15 | 100.00    | 1077.3 |
| 343.15 | 10000.00  | 1148.0 |
| 343.15 | 20000.00  | 1211.1 |
| 343.15 | 30000.00  | 1268.5 |
| 343.15 | 40000.00  | 1321.7 |
| 343.15 | 50000.00  | 1370.5 |
| 343.15 | 60000.00  | 1416.0 |
| 343.15 | 70000.00  | 1458.4 |
| 343.15 | 80000.00  | 1499.4 |
| 343.15 | 90000.00  | 1537.9 |
| 343.15 | 100000.00 | 1574.6 |
| 353.15 | 100.00    | 1037.7 |
| 353.15 | 10000.00  | 1111.6 |
| 353.15 | 20000.00  | 1177.7 |
| 353.15 | 30000.00  | 1236.9 |
| 353.15 | 40000.00  | 1291.4 |
| 353.15 | 50000.00  | 1342.1 |
| 353.15 | 60000.00  | 1387.8 |
| 353.15 | 70000.00  | 1431.2 |
| 353.15 | 80000.00  | 1472.7 |
| 353.15 | 90000.00  | 1511.9 |
| 353.15 | 100000.00 | 1549.3 |
| 363.15 | 100.00    | 998.2  |
| 363.15 | 10000.00  | 1076.2 |
| 363.15 | 20000.00  | 1144.6 |
| 363.15 | 30000.00  | 1205.4 |
| 363.15 | 40000.00  | 1261.4 |
| 363.15 | 50000.00  | 1312.6 |
| 363.15 | 60000.00  | 1359.8 |
| 363.15 | 70000.00  | 1404.8 |
| 363.15 | 80000.00  | 1446.9 |
| 363.15 | 90000.00  | 1486.5 |
| 363.15 | 100000.00 | 1524.4 |
| 373.15 | 100.00    | 957.7  |
| 373.15 | 10000.00  | 1039.5 |

|           |           |                                                                                                           |
|-----------|-----------|-----------------------------------------------------------------------------------------------------------|
| 373.15    | 20000.00  | 1110.9                                                                                                    |
| 373.15    | 30000.00  | 1174.0                                                                                                    |
| 373.15    | 40000.00  | 1231.1                                                                                                    |
| 373.15    | 50000.00  | 1283.7                                                                                                    |
| 373.15    | 60000.00  | 1332.0                                                                                                    |
| 373.15    | 70000.00  | 1377.5                                                                                                    |
| 373.15    | 80000.00  | 1420.3                                                                                                    |
| 373.15    | 90000.00  | 1461.1                                                                                                    |
| 373.15    | 100000.00 | 1499.3                                                                                                    |
| Reference |           | <a href="https://www.doi.org/10.1016/j.jct.2005.10.002">https://www.doi.org/10.1016/j.jct.2005.10.002</a> |

## Sources

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<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Study of the volumetric properties of weakly associated alcohols by means of high speed of sound measurements:  
Aqueous Solubility Prediction Method:

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[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
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Estimated Solubility Method:

[http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C77747&Units=SI>

## 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>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>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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