

# Benzene, 1-methyl-3-propyl-

|                      |                                                              |
|----------------------|--------------------------------------------------------------|
| Other names:         | 1-Methyl-3-n-propylbenzene                                   |
|                      | 1-Methyl-3-propylbenzene                                     |
|                      | 3-Propyl-toluene                                             |
|                      | 3-n-Propyltoluene                                            |
|                      | M-METHYLPROPYLBENZENE                                        |
|                      | M-PROPYLTOLUENE                                              |
|                      | Toluene, m-propyl-                                           |
| Inchi:               | InChI=1S/C10H14/c1-3-5-10-7-4-6-9(2)8-10/h4,6-8H,3,5H2,1-2H3 |
| InchiKey:            | QUEBYVKXYIKVSO-UHFFFAOYSA-N                                  |
| Formula:             | C10H14                                                       |
| SMILES:              | CCc1cccc(C)c1                                                |
| Mol. weight [g/mol]: | 134.22                                                       |
| CAS:                 | 1074-43-7                                                    |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| af            | 0.4120          |        | KDB            |
| chl           | -5859.70 ± 1.10 | kJ/mol | NIST Webbook   |
| chl           | -5860.60 ± 2.20 | kJ/mol | NIST Webbook   |
| gf            | 136.10          | kJ/mol | Joback Method  |
| hf            | -24.67          | kJ/mol | Joback Method  |
| hfl           | -75.40 ± 2.20   | kJ/mol | NIST Webbook   |
| hfl           | -76.20 ± 1.20   | kJ/mol | NIST Webbook   |
| hfus          | 15.31           | kJ/mol | Joback Method  |
| hvap          | 52.10           | kJ/mol | NIST Webbook   |
| log10ws       | -3.17           |        | Crippen Method |
| logp          | 2.948           |        | Crippen Method |
| mcvol         | 128.000         | ml/mol | McGowan Method |
| pc            | 2904.00         | kPa    | KDB            |
| rinpol        | 1034.00         |        | NIST Webbook   |
| rinpol        | 1043.00         |        | NIST Webbook   |
| rinpol        | 1034.80         |        | NIST Webbook   |
| rinpol        | 1043.00         |        | NIST Webbook   |
| rinpol        | 1048.00         |        | NIST Webbook   |
| rinpol        | 1043.00         |        | NIST Webbook   |
| rinpol        | 1030.40         |        | NIST Webbook   |
| rinpol        | 1032.80         |        | NIST Webbook   |

|        |         |              |
|--------|---------|--------------|
| rinpol | 1043.40 | NIST Webbook |
| rinpol | 1048.20 | NIST Webbook |
| rinpol | 1054.40 | NIST Webbook |
| rinpol | 1031.60 | NIST Webbook |
| rinpol | 1027.80 | NIST Webbook |
| rinpol | 1030.40 | NIST Webbook |
| rinpol | 1032.80 | NIST Webbook |
| rinpol | 1027.78 | NIST Webbook |
| rinpol | 1051.00 | NIST Webbook |
| rinpol | 1056.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1057.00 | NIST Webbook |
| rinpol | 1060.00 | NIST Webbook |
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| rinpol | 1063.00 | NIST Webbook |
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| rinpol | 1030.50 | NIST Webbook |
| rinpol | 1065.30 | NIST Webbook |
| rinpol | 1036.00 | NIST Webbook |
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| rinpol | 1037.00 | NIST Webbook |
| rinpol | 1037.02 | NIST Webbook |
| rinpol | 1037.76 | NIST Webbook |
| rinpol | 1038.00 | NIST Webbook |
| rinpol | 1037.58 | NIST Webbook |
| rinpol | 1036.00 | NIST Webbook |
| rinpol | 1057.61 | NIST Webbook |
| rinpol | 1043.00 | NIST Webbook |

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| rinpol | 1043.00 | NIST Webbook |
| rinpol | 1048.00 | NIST Webbook |
| rinpol | 1048.00 | NIST Webbook |
| rinpol | 1024.00 | NIST Webbook |
| rinpol | 1036.00 | NIST Webbook |
| rinpol | 1041.00 | NIST Webbook |
| rinpol | 1003.00 | NIST Webbook |
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| rinpol | 1042.00 | NIST Webbook |
| rinpol | 1052.00 | NIST Webbook |
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| rinpol | 1037.58 | NIST Webbook |
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| rinpol | 1042.00 | NIST Webbook |
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|-------|---------------|---------|---------------|
| ripol | 1032.00       |         | NIST Webbook  |
| ripol | 1040.60       |         | NIST Webbook  |
| ripol | 1032.00       |         | NIST Webbook  |
| ripol | 1054.00       |         | NIST Webbook  |
| ripol | 1262.00       |         | NIST Webbook  |
| ripol | 1297.00       |         | NIST Webbook  |
| ripol | 1284.00       |         | NIST Webbook  |
| ripol | 1277.00       |         | NIST Webbook  |
| ripol | 1301.00       |         | NIST Webbook  |
| ripol | 1277.00       |         | NIST Webbook  |
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| ripol | 1354.00       |         | NIST Webbook  |
| ripol | 1338.00       |         | NIST Webbook  |
| ripol | 1326.00       |         | NIST Webbook  |
| ripol | 1315.00       |         | NIST Webbook  |
| ripol | 1314.00       |         | NIST Webbook  |
| ripol | 1297.00       |         | NIST Webbook  |
| ripol | 1277.20       |         | NIST Webbook  |
| ripol | 1277.20       |         | NIST Webbook  |
| ripol | 1301.00       |         | NIST Webbook  |
| ripol | 1301.00       |         | NIST Webbook  |
| ripol | 1259.00       |         | NIST Webbook  |
| ripol | 1259.00       |         | NIST Webbook  |
| tb    | 455.20        | K       | NIST Webbook  |
| tb    | 455.20        | K       | KDB           |
| tb    | 450.20 ± 3.00 | K       | NIST Webbook  |
| tb    | 451.00 ± 5.00 | K       | NIST Webbook  |
| tb    | 451.00 ± 5.00 | K       | NIST Webbook  |
| tb    | 454.90 ± 0.40 | K       | NIST Webbook  |
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| tb    | 454.90 ± 0.40 | K       | NIST Webbook  |
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| tb    | 454.90 ± 0.40 | K       | NIST Webbook  |
| tb    | 453.00 ± 2.00 | K       | NIST Webbook  |
| tb    | 455.21 ± 0.20 | K       | NIST Webbook  |
| tb    | 455.13 ± 0.30 | K       | NIST Webbook  |
| tb    | 455.21 ± 0.20 | K       | NIST Webbook  |
| tb    | 455.20 ± 0.20 | K       | NIST Webbook  |
| tb    | 455.15 ± 0.50 | K       | NIST Webbook  |
| tc    | 666.60        | K       | KDB           |
| tf    | 190.57 ± 0.02 | K       | NIST Webbook  |
| vc    | 0.487         | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 257.29    | J/mol×K | 459.86          | Joback Method |
| cpg           | 271.96    | J/mol×K | 494.18          | Joback Method |
| cpg           | 285.87    | J/mol×K | 528.50          | Joback Method |
| cpg           | 299.03    | J/mol×K | 562.82          | Joback Method |
| cpg           | 311.49    | J/mol×K | 597.14          | Joback Method |
| cpg           | 323.27    | J/mol×K | 631.46          | Joback Method |
| cpg           | 334.39    | J/mol×K | 665.78          | Joback Method |
| dvisc         | 0.0012559 | Pa×s    | 277.81          | Joback Method |
| dvisc         | 0.0024545 | Pa×s    | 241.40          | Joback Method |
| dvisc         | 0.0007506 | Pa×s    | 314.22          | Joback Method |
| dvisc         | 0.0004992 | Pa×s    | 350.63          | Joback Method |
| dvisc         | 0.0003585 | Pa×s    | 387.04          | Joback Method |
| dvisc         | 0.0002725 | Pa×s    | 423.45          | Joback Method |
| dvisc         | 0.0002163 | Pa×s    | 459.86          | Joback Method |
| hvapt         | 47.80     | kJ/mol  | 409.50          | NIST Webbook  |
| rhoI          | 859.01    | kg/m3   | 293.10          | KDB           |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.44657e+01                   |
| Coeff. B                    | -3.84928e+03                  |
| Coeff. C                    | -6.40540e+01                  |
| Temperature range (K), min. | 335.55                        |
| Temperature range (K), max. | 484.55                        |

| Information   | Value                                      |
|---------------|--------------------------------------------|
| Property code | pvap                                       |
| Equation      | $\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$ |
| Coeff. A      | 1.05651e+02                                |
| Coeff. B      | -9.71981e+03                               |
| Coeff. C      | -1.32760e+01                               |

|                             |             |
|-----------------------------|-------------|
| Coeff. D                    | 7.64429e-06 |
| Temperature range (K), min. | 334.15      |
| Temperature range (K), max. | 485.15      |

## Sources

|                                             |                                                                                                                                                                                         |
|---------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b>                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| <b>NIST Webbook:</b>                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074437&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074437&amp;Units=SI</a>                                             |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| <b>KDB Vapor Pressure Data:</b>             | <a href="https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=670">https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=670</a>                                       |
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                                                               |
| <b>Crippen Method:</b>                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| <b>Joback Method:</b>                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| <b>KDB:</b>                                 | <a href="https://www.cheric.org/files/research/kdb/mol/mol670.mol">https://www.cheric.org/files/research/kdb/mol/mol670.mol</a>                                                         |

## Legend

|                 |                                                           |
|-----------------|-----------------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                           |
| <b>chl:</b>     | Standard liquid enthalpy of combustion                    |
| <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>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>rho:</b>     | Liquid Density                                            |
| <b>rinpol:</b>  | Non-polar retention indices                               |
| <b>ripol:</b>   | Polar retention indices                                   |
| <b>tb:</b>      | Normal Boiling Point Temperature                          |
| <b>tc:</b>      | Critical Temperature                                      |
| <b>tf:</b>      | Normal melting (fusion) point                             |

**vc:** Critical Volume

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<https://www.chemeo.com/cid/49-867-6/Benzene-1-methyl-3-propyl.pdf>

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