

# Benzene, decyl-

|                      |                                                                                    |
|----------------------|------------------------------------------------------------------------------------|
| Other names:         | 1-PHENYLDECANE<br>DECYLBENZENE<br>Decane, 1-phenyl-<br>n-Decylbenzene              |
| Inchi:               | InChI=1S/C16H26/c1-2-3-4-5-6-7-8-10-13-16-14-11-9-12-15-16/h9,11-12,14-15H,2-8,10, |
| InchiKey:            | UZILCZKGXMQEQR-UHFFFAOYSA-N                                                        |
| Formula:             | C16H26                                                                             |
| SMILES:              | CCCCCCCCCc1ccccc1                                                                  |
| Mol. weight [g/mol]: | 218.38                                                                             |
| CAS:                 | 104-72-3                                                                           |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| af            | 0.6750          |        | KDB            |
| chl           | -9796.30 ± 3.70 | kJ/mol | NIST Webbook   |
| chl           | -9793.00 ± 1.80 | kJ/mol | NIST Webbook   |
| gf            | 196.25          | kJ/mol | Joback Method  |
| hf            | -137.04         | kJ/mol | Joback Method  |
| hfl           | -219.10 ± 2.00  | kJ/mol | NIST Webbook   |
| hfus          | 31.24           | kJ/mol | Joback Method  |
| hvap          | 78.20 ± 0.30    | kJ/mol | NIST Webbook   |
| hvap          | 79.80           | kJ/mol | NIST Webbook   |
| log10ws       | -5.62           |        | Crippen Method |
| logp          | 5.370           |        | Crippen Method |
| mcvol         | 212.540         | ml/mol | McGowan Method |
| nfpaf         | %!d(float64=1)  |        | KDB            |
| nfpah         | %!d(float64=2)  |        | KDB            |
| pc            | 1780.00         | kPa    | KDB            |
| rinpol        | 1661.14         |        | NIST Webbook   |
| rinpol        | 1677.70         |        | NIST Webbook   |
| rinpol        | 1674.80         |        | NIST Webbook   |
| rinpol        | 1674.50         |        | NIST Webbook   |
| rinpol        | 1664.00         |        | NIST Webbook   |
| rinpol        | 1655.82         |        | NIST Webbook   |
| rinpol        | 1674.80         |        | NIST Webbook   |
| rinpol        | 1664.63         |        | NIST Webbook   |
| rinpol        | 1675.02         |        | NIST Webbook   |

|        |               |         |               |
|--------|---------------|---------|---------------|
| rinpol | 1680.77       |         | NIST Webbook  |
| rinpol | 1684.34       |         | NIST Webbook  |
| rinpol | 1659.00       |         | NIST Webbook  |
| rinpol | 1659.00       |         | NIST Webbook  |
| rinpol | 1669.50       |         | NIST Webbook  |
| rinpol | 1627.00       |         | NIST Webbook  |
| rinpol | 280.90        |         | NIST Webbook  |
| rinpol | 284.70        |         | NIST Webbook  |
| rinpol | 1659.00       |         | NIST Webbook  |
| rinpol | 1645.00       |         | NIST Webbook  |
| rinpol | 1677.70       |         | NIST Webbook  |
| rinpol | 1674.80       |         | NIST Webbook  |
| rinpol | 1669.50       |         | NIST Webbook  |
| rinpol | 1674.50       |         | NIST Webbook  |
| rinpol | 1674.80       |         | NIST Webbook  |
| rinpol | 1694.00       |         | NIST Webbook  |
| rinpol | 1655.00       |         | NIST Webbook  |
| rinpol | 1627.00       |         | NIST Webbook  |
| rinpol | 1664.00       |         | NIST Webbook  |
| rinpol | 1659.00       |         | NIST Webbook  |
| ripol  | 1928.00       |         | NIST Webbook  |
| ripol  | 1928.00       |         | NIST Webbook  |
| ripol  | 1953.00       |         | NIST Webbook  |
| ripol  | 1962.00       |         | NIST Webbook  |
| ripol  | 1928.00       |         | NIST Webbook  |
| sg     | 674.00 ± 2.10 | J/mol×K | NIST Webbook  |
| tb     | 571.10        | K       | KDB           |
| tb     | 566.20        | K       | NIST Webbook  |
| tc     | 753.00        | K       | KDB           |
| tf     | 259.00        | K       | KDB           |
| tt     | 258.75 ± 0.02 | K       | NIST Webbook  |
| vc     | 0.824         | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 544.76 | J/mol×K | 592.16          | Joback Method |
| cpg           | 563.84 | J/mol×K | 623.71          | Joback Method |
| cpg           | 581.93 | J/mol×K | 655.26          | Joback Method |
| cpg           | 599.08 | J/mol×K | 686.81          | Joback Method |
| cpg           | 615.32 | J/mol×K | 718.36          | Joback Method |

|       |           |         |        |                                                                                            |
|-------|-----------|---------|--------|--------------------------------------------------------------------------------------------|
| cpg   | 630.68    | J/mol×K | 749.91 | Joback Method                                                                              |
| cpg   | 645.22    | J/mol×K | 781.46 | Joback Method                                                                              |
| dvisc | 0.0034038 | Pa×s    | 296.50 | Joback Method                                                                              |
| dvisc | 0.0013986 | Pa×s    | 345.78 | Joback Method                                                                              |
| dvisc | 0.0007175 | Pa×s    | 395.05 | Joback Method                                                                              |
| dvisc | 0.0004268 | Pa×s    | 444.33 | Joback Method                                                                              |
| dvisc | 0.0002816 | Pa×s    | 493.61 | Joback Method                                                                              |
| dvisc | 0.0002004 | Pa×s    | 542.88 | Joback Method                                                                              |
| dvisc | 0.0001509 | Pa×s    | 592.16 | Joback Method                                                                              |
| hvapt | 61.60     | kJ/mol  | 523.00 | NIST Webbook                                                                               |
| hvapt | 78.00     | kJ/mol  | 373.00 | NIST Webbook                                                                               |
| hvapt | 75.10     | kJ/mol  | 399.00 | NIST Webbook                                                                               |
| hvapt | 50.63     | kJ/mol  | 571.10 | KDB                                                                                        |
| pvap  | 1.22e-03  | kPa     | 318.20 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap  | 1.92e-03  | kPa     | 323.20 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap  | 2.93e-03  | kPa     | 328.30 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap  | 4.50e-03  | kPa     | 333.50 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap  | 6.55e-03  | kPa     | 338.60 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap  | 9.66e-03  | kPa     | 343.70 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |

|      |      |     |        |                                                                                            |
|------|------|-----|--------|--------------------------------------------------------------------------------------------|
| pvap | 0.01 | kPa | 348.70 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap | 0.02 | kPa | 353.30 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap | 0.03 | kPa | 358.40 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |
| pvap | 0.04 | kPa | 363.40 | Vapour pressures and enthalpies of vaporization of a series of the linear n-alkyl-benzenes |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.52519e+01                   |
| Coeff. B                    | -5.25804e+03                  |
| Coeff. C                    | -7.65640e+01                  |
| Temperature range (K), min. | 427.94                        |
| Temperature range (K), max. | 605.52                        |

| Information                 | Value                                      |
|-----------------------------|--------------------------------------------|
| Property code               | pvap                                       |
| Equation                    | $\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$ |
| Coeff. A                    | 1.30338e+02                                |
| Coeff. B                    | -1.40293e+04                               |
| Coeff. C                    | -1.62264e+01                               |
| Coeff. D                    | 5.67144e-06                                |
| Temperature range (K), min. | 258.77                                     |

Datasets

Mass density, kg/m3

| Temperature, K - Liquid | Pressure, kPa - Liquid | Mass density, kg/m3 - Liquid |
|-------------------------|------------------------|------------------------------|
| 293.15                  | 100.00                 | 855.8                        |
| 293.15                  | 5000.00                | 858.6                        |
| 293.15                  | 10000.00               | 861.5                        |
| 293.15                  | 15000.00               | 864.2                        |
| 293.15                  | 20000.00               | 867.0                        |
| 293.15                  | 25000.00               | 869.5                        |
| 293.15                  | 30000.00               | 872.0                        |
| 293.15                  | 35000.00               | 874.4                        |
| 293.15                  | 40000.00               | 876.8                        |
| 293.15                  | 45000.00               | 879.0                        |
| 293.15                  | 50000.00               | 881.4                        |
| 293.15                  | 55000.00               | 883.5                        |
| 293.15                  | 60000.00               | 885.7                        |
| 293.15                  | 65000.00               | 887.8                        |
| 303.15                  | 100.00                 | 849.1                        |
| 303.15                  | 5000.00                | 852.2                        |
| 303.15                  | 10000.00               | 855.1                        |
| 303.15                  | 15000.00               | 858.2                        |
| 303.15                  | 20000.00               | 860.9                        |
| 303.15                  | 25000.00               | 863.6                        |
| 303.15                  | 30000.00               | 866.2                        |
| 303.15                  | 35000.00               | 868.7                        |
| 303.15                  | 40000.00               | 871.2                        |
| 303.15                  | 45000.00               | 873.5                        |
| 303.15                  | 50000.00               | 875.9                        |
| 303.15                  | 55000.00               | 878.2                        |
| 303.15                  | 60000.00               | 880.4                        |
| 303.15                  | 65000.00               | 882.6                        |
| 313.15                  | 100.00                 | 842.1                        |
| 313.15                  | 5000.00                | 845.3                        |
| 313.15                  | 10000.00               | 848.4                        |
| 313.15                  | 15000.00               | 851.3                        |

|        |          |       |
|--------|----------|-------|
| 313.15 | 20000.00 | 854.1 |
| 313.15 | 25000.00 | 856.9 |
| 313.15 | 30000.00 | 859.7 |
| 313.15 | 35000.00 | 862.3 |
| 313.15 | 40000.00 | 864.9 |
| 313.15 | 45000.00 | 867.4 |
| 313.15 | 50000.00 | 869.9 |
| 313.15 | 55000.00 | 872.2 |
| 313.15 | 60000.00 | 874.6 |
| 313.15 | 65000.00 | 876.8 |
| 323.15 | 100.00   | 835.1 |
| 323.15 | 5000.00  | 838.3 |
| 323.15 | 10000.00 | 841.6 |
| 323.15 | 15000.00 | 844.6 |
| 323.15 | 20000.00 | 847.7 |
| 323.15 | 25000.00 | 850.8 |
| 323.15 | 30000.00 | 853.6 |
| 323.15 | 35000.00 | 856.3 |
| 323.15 | 40000.00 | 859.0 |
| 323.15 | 45000.00 | 861.5 |
| 323.15 | 50000.00 | 864.1 |
| 323.15 | 55000.00 | 866.6 |
| 323.15 | 60000.00 | 868.9 |
| 323.15 | 65000.00 | 871.2 |
| 333.15 | 100.00   | 827.8 |
| 333.15 | 5000.00  | 831.3 |
| 333.15 | 10000.00 | 834.9 |
| 333.15 | 15000.00 | 838.2 |
| 333.15 | 20000.00 | 841.3 |
| 333.15 | 25000.00 | 844.3 |
| 333.15 | 30000.00 | 847.2 |
| 333.15 | 35000.00 | 850.1 |
| 333.15 | 40000.00 | 852.8 |
| 333.15 | 45000.00 | 855.5 |
| 333.15 | 50000.00 | 858.1 |
| 333.15 | 55000.00 | 860.8 |
| 333.15 | 60000.00 | 863.2 |
| 333.15 | 65000.00 | 865.7 |
| 343.15 | 100.00   | 821.0 |
| 343.15 | 5000.00  | 824.6 |
| 343.15 | 10000.00 | 828.2 |
| 343.15 | 15000.00 | 831.6 |
| 343.15 | 20000.00 | 834.9 |
| 343.15 | 25000.00 | 838.1 |

|        |          |       |
|--------|----------|-------|
| 343.15 | 30000.00 | 841.1 |
| 343.15 | 35000.00 | 844.0 |
| 343.15 | 40000.00 | 846.8 |
| 343.15 | 45000.00 | 849.8 |
| 343.15 | 50000.00 | 852.4 |
| 343.15 | 55000.00 | 855.1 |
| 343.15 | 60000.00 | 857.6 |
| 343.15 | 65000.00 | 860.1 |
| 353.15 | 100.00   | 814.0 |
| 353.15 | 5000.00  | 817.8 |
| 353.15 | 10000.00 | 821.5 |
| 353.15 | 15000.00 | 825.2 |
| 353.15 | 20000.00 | 828.7 |
| 353.15 | 25000.00 | 831.9 |
| 353.15 | 30000.00 | 835.0 |
| 353.15 | 35000.00 | 838.1 |
| 353.15 | 40000.00 | 841.0 |
| 353.15 | 45000.00 | 843.9 |
| 353.15 | 50000.00 | 846.6 |
| 353.15 | 55000.00 | 849.4 |
| 353.15 | 60000.00 | 852.0 |
| 353.15 | 65000.00 | 854.7 |

Reference

<https://www.doi.org/10.1021/je0500936>

Sources

Vapour pressures and enthalpies of vaporization of a series of the linear n-alkanes: Properties of 1-Phenyldecane and 1-Phenylundecane at Pressures to 65 MPa and Temperature between 293.15 and 593.15 K.
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# 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>nfpaf:</b>   | NFPA Fire Rating                                          |
| <b>nfpah:</b>   | NFPA Health Rating                                        |
| <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>sg:</b>      | Molar entropy at standard conditions                      |
| <b>tb:</b>      | Normal Boiling Point Temperature                          |
| <b>tc:</b>      | Critical Temperature                                      |
| <b>tf:</b>      | Normal melting (fusion) point                             |
| <b>tt:</b>      | Triple Point Temperature                                  |
| <b>vc:</b>      | Critical Volume                                           |

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