

n-Heptadecylbenzene

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|-----------------------------|--|
| Other names: | 1-Phenylheptadecane Benzene, heptadecyl- Heptadecylbenzene heptadecane, 1-phenyl- |
| Inchi: | InChI=1S/C23H40/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23-21-18-16-19-22-23/h |
| InchiKey: | ZMPPFNHWMJARX-UHFFFAOYSA-N |
| Formula: | C23H40 |
| SMILES: | CCCCCCCCCCCCCCCCc1ccccc1 |
| Mol. weight [g/mol]: | 316.56 |
| CAS: | 14752-75-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| gf | 255.19 | kJ/mol | Joback Method |
| hf | -281.52 | kJ/mol | Joback Method |
| hfus | 49.37 | kJ/mol | Joback Method |
| hvap | 69.07 | kJ/mol | Joback Method |
| log10ws | -8.55 | | Crippen Method |
| logp | 8.101 | | Crippen Method |
| mcvol | 311.170 | ml/mol | McGowan Method |
| pc | 1043.95 | kPa | Joback Method |
| tb | 752.32 | K | Joback Method |
| tc | 935.08 | K | Joback Method |
| tf | 311.00 ± 2.00 | K | NIST Webbook |
| vc | 1.216 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1056.00 | J/mol×K | 935.08 | Joback Method |
| cpg | 945.69 | J/mol×K | 752.32 | Joback Method |
| cpg | 966.62 | J/mol×K | 782.78 | Joback Method |
| cpg | 986.46 | J/mol×K | 813.24 | Joback Method |
| cpg | 1005.27 | J/mol×K | 843.70 | Joback Method |

| | | | | |
|-------|-----------|---------|--------|---------------|
| cpg | 1023.10 | J/molxK | 874.16 | Joback Method |
| cpg | 1039.99 | J/molxK | 904.62 | Joback Method |
| dvisc | 0.0000671 | Paxs | 752.32 | Joback Method |
| dvisc | 0.0019107 | Paxs | 375.39 | Joback Method |
| dvisc | 0.0007328 | Paxs | 438.21 | Joback Method |
| dvisc | 0.0003574 | Paxs | 501.03 | Joback Method |
| dvisc | 0.0002045 | Paxs | 563.86 | Joback Method |
| dvisc | 0.0001309 | Paxs | 626.68 | Joback Method |
| dvisc | 0.0000909 | Paxs | 689.50 | Joback Method |
| hvapt | 98.50 | kJ/mol | 539.00 | NIST Webbook |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--|
| tfp | 292.80 | K | 100.00 | Solid-Liquid Equilibria under High Pressure of Nine Pure n-Alkylbenzenes |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.41856e+01 |
| Coeff. B | -4.87150e+03 |
| Coeff. C | -1.54932e+02 |
| Temperature range (K), min. | 505.45 |
| Temperature range (K), max. | 703.89 |

Datasets

Speed of sound, m/s

| Pressure, kPa - Liquid | Temperature, K - Liquid | Speed of sound, m/s - Liquid |
|------------------------|-------------------------|------------------------------|
| 100.00 | 303.15 | 1422.6 |
| 100.00 | 313.15 | 1387.1 |
| 100.00 | 323.15 | 1352.6 |
| 100.00 | 333.15 | 1319.9 |
| 100.00 | 343.15 | 1287.0 |
| 100.00 | 353.15 | 1255.2 |
| 100.00 | 363.15 | 1223.6 |
| 100.00 | 373.15 | 1193.0 |
| 10000.00 | 303.15 | 1467.5 |
| 10000.00 | 313.15 | 1433.6 |
| 10000.00 | 323.15 | 1402.3 |
| 10000.00 | 333.15 | 1370.2 |
| 10000.00 | 343.15 | 1338.7 |
| 10000.00 | 353.15 | 1308.6 |
| 10000.00 | 363.15 | 1278.7 |
| 10000.00 | 373.15 | 1249.5 |
| 20000.00 | 303.15 | 1510.9 |
| 20000.00 | 313.15 | 1479.2 |
| 20000.00 | 323.15 | 1447.9 |
| 20000.00 | 333.15 | 1417.3 |
| 20000.00 | 343.15 | 1387.3 |
| 20000.00 | 353.15 | 1359.3 |
| 20000.00 | 363.15 | 1330.3 |
| 20000.00 | 373.15 | 1302.6 |
| 30000.00 | 303.15 | 1552.0 |
| 30000.00 | 313.15 | 1520.4 |
| 30000.00 | 323.15 | 1490.8 |
| 30000.00 | 333.15 | 1461.4 |
| 30000.00 | 343.15 | 1432.3 |
| 30000.00 | 353.15 | 1405.3 |
| 30000.00 | 363.15 | 1378.0 |
| 30000.00 | 373.15 | 1351.4 |
| 40000.00 | 303.15 | 1590.5 |
| 40000.00 | 313.15 | 1559.7 |
| 40000.00 | 323.15 | 1531.1 |
| 40000.00 | 333.15 | 1502.9 |
| 40000.00 | 343.15 | 1475.5 |
| 40000.00 | 353.15 | 1448.5 |
| 40000.00 | 363.15 | 1422.2 |

| | | |
|-----------|--------|--------|
| 40000.00 | 373.15 | 1396.8 |
| 50000.00 | 303.15 | 1627.2 |
| 50000.00 | 313.15 | 1597.9 |
| 50000.00 | 323.15 | 1569.2 |
| 50000.00 | 333.15 | 1542.1 |
| 50000.00 | 343.15 | 1515.3 |
| 50000.00 | 353.15 | 1489.5 |
| 50000.00 | 363.15 | 1464.0 |
| 50000.00 | 373.15 | 1439.2 |
| 60000.00 | 303.15 | 1661.9 |
| 60000.00 | 313.15 | 1633.6 |
| 60000.00 | 323.15 | 1605.8 |
| 60000.00 | 333.15 | 1579.2 |
| 60000.00 | 343.15 | 1553.3 |
| 60000.00 | 353.15 | 1528.3 |
| 60000.00 | 363.15 | 1503.3 |
| 60000.00 | 373.15 | 1479.7 |
| 70000.00 | 303.15 | 1695.6 |
| 70000.00 | 313.15 | 1667.3 |
| 70000.00 | 323.15 | 1640.7 |
| 70000.00 | 333.15 | 1614.6 |
| 70000.00 | 343.15 | 1589.5 |
| 70000.00 | 353.15 | 1564.8 |
| 70000.00 | 363.15 | 1541.1 |
| 70000.00 | 373.15 | 1517.7 |
| 80000.00 | 313.15 | 1700.0 |
| 80000.00 | 323.15 | 1673.9 |
| 80000.00 | 333.15 | 1648.7 |
| 80000.00 | 343.15 | 1624.1 |
| 80000.00 | 353.15 | 1600.1 |
| 80000.00 | 363.15 | 1576.4 |
| 80000.00 | 373.15 | 1553.8 |
| 90000.00 | 313.15 | 1731.8 |
| 90000.00 | 323.15 | 1705.8 |
| 90000.00 | 333.15 | 1681.3 |
| 90000.00 | 343.15 | 1657.2 |
| 90000.00 | 353.15 | 1633.4 |
| 90000.00 | 363.15 | 1610.7 |
| 90000.00 | 373.15 | 1588.6 |
| 100000.00 | 313.15 | 1762.0 |
| 100000.00 | 323.15 | 1736.6 |
| 100000.00 | 333.15 | 1712.2 |
| 100000.00 | 343.15 | 1688.0 |
| 100000.00 | 353.15 | 1665.5 |

| | | |
|-----------|--------|--------|
| 100000.00 | 363.15 | 1643.4 |
| 100000.00 | 373.15 | 1621.8 |
| 110000.00 | 313.15 | 1790.2 |
| 110000.00 | 323.15 | 1766.3 |
| 110000.00 | 333.15 | 1742.3 |
| 110000.00 | 343.15 | 1719.2 |
| 110000.00 | 353.15 | 1696.9 |
| 110000.00 | 363.15 | 1674.6 |
| 110000.00 | 373.15 | 1653.6 |
| 120000.00 | 313.15 | 1818.7 |
| 120000.00 | 323.15 | 1794.9 |
| 120000.00 | 333.15 | 1771.7 |
| 120000.00 | 343.15 | 1748.7 |
| 120000.00 | 353.15 | 1726.9 |
| 120000.00 | 363.15 | 1705.0 |
| 120000.00 | 373.15 | 1684.3 |
| 130000.00 | 313.15 | 1847.1 |
| 130000.00 | 323.15 | 1822.8 |
| 130000.00 | 333.15 | 1799.8 |
| 130000.00 | 343.15 | 1777.4 |
| 130000.00 | 353.15 | 1755.8 |
| 130000.00 | 363.15 | 1734.4 |
| 130000.00 | 373.15 | 1713.8 |
| 140000.00 | 323.15 | 1849.3 |
| 140000.00 | 333.15 | 1826.9 |
| 140000.00 | 343.15 | 1805.0 |
| 140000.00 | 353.15 | 1783.8 |
| 140000.00 | 363.15 | 1763.3 |
| 140000.00 | 373.15 | 1742.7 |
| 150000.00 | 323.15 | 1875.5 |
| 150000.00 | 333.15 | 1853.6 |
| 150000.00 | 343.15 | 1832.0 |
| 150000.00 | 353.15 | 1811.1 |
| 150000.00 | 363.15 | 1790.0 |
| 150000.00 | 373.15 | 1770.5 |

Reference

<https://www.doi.org/10.1021/je049973v>

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C14752751&Units=SI>

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|---|---|
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Speed of Sound, Density, and Compressibility of Alkyl-Benzenes as a Solid, Liquid, Gas, and Temperature: | https://www.doi.org/10.1021/je049973v |
| Pressure of Nine Pure and Octadecylbenzene: | https://www.doi.org/10.1021/je700529y |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

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|-----------------|---|
| cpg: | Ideal gas 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 |
| hvap: | Enthalpy of vaporization at standard conditions |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pvap: | Vapor pressure |
| speedsl: | Speed of sound in fluid |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| tfp: | Melting point |
| vc: | Critical Volume |

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