# Benzene, 1-(1,1-dimethylethyl)-3,5-dimethyl-

| | |
|---|---|
| **Other names:** | 1,3-Dimethyl-5-tert-butylbenzene |
| | 1-tert-Butyl-3,5-dimethylbenzene |
| | 1-tert-Butyl-3,5-dimethylbezene |
| | 4-tert-Butyl-2,6-dimethylbenzene |
| | 5-tert-Butyl-1,3-dimethylbenzene |
| | 5-tert-Butyl-m-xylene |
| | Benzene, 1,3-dimethyl-5-(1,1-dimethylethyl) |
| | Benzene, 1,3-dimethyl-5-tert-butyl |
| | Benzene, 5-tert-butyl-1,3-dimethyl- |
| | NSC 11016 |
| | m-Xylene, 5-tert-butyl- |
| **Inchi:** | InChI=1S/C12H18/c1-9-6-10(2)8-11(7-9)12(3,4)5/h6-8H,1-5H3 |
| **InchiKey:** | FZSPYHREEHYLCB-UHFFFAOYSA-N |
| **Formula:** | C12H18 |
| **SMILES:** | Cc1cc(C)cc(C(C)(C)C)c1 |
| **Mol. weight [g/mol]:** | 162.27 |
| **CAS:** | 98-19-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 146.15 | kJ/mol | Joback Method |
| hf | -86.17 | kJ/mol | Joback Method |
| hfus | 12.69 | kJ/mol | Joback Method |
| hvap | 56.60 ± 0.60 | kJ/mol | NIST Webbook |
| log10ws | -3.74 | | Crippen Method |
| logp | 3.601 | | Crippen Method |
| mcvol | 156.180 | ml/mol | McGowan Method |
| pc | 2379.54 | kPa | Joback Method |
| rinpol | 1165.20 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1163.00 | | NIST Webbook |
| rinpol | 1169.60 | | NIST Webbook |
| rinpol | 1163.60 | | NIST Webbook |
| rinpol | 1146.85 | | NIST Webbook |
| rinpol | 1151.00 | | NIST Webbook |
| rinpol | 1165.00 | | NIST Webbook |
| rinpol | 1163.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 1160.00 | | NIST Webbook |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1169.00 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1163.60 | | NIST Webbook |
| rinpol | 1160.00 | | NIST Webbook |
| rinpol | 1169.00 | | NIST Webbook |
| rinpol | 1164.00 | | NIST Webbook |
| rinpol | 1160.00 | | NIST Webbook |
| ripol | 1430.80 | | NIST Webbook |
| ripol | 1385.00 | | NIST Webbook |
| ripol | 1385.00 | | NIST Webbook |
| ripol | 1385.00 | | NIST Webbook |
| ripol | 1391.40 | | NIST Webbook |
| tb | 482.00 ± 1.50 | K | NIST Webbook |
| tb | 478.70 | K | NIST Webbook |
| tb | 475.00 | K | NIST Webbook |
| tc | 722.03 | K | Joback Method |
| tf | 254.90 ± 1.50 | K | NIST Webbook |
| vc | 0.589 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 426.96 | J/mol×K | 686.25 | Joback Method |
| cpg | 439.68 | J/mol×K | 722.03 | Joback Method |
| cpg | 349.74 | J/mol×K | 507.37 | Joback Method |
| cpg | 367.17 | J/mol×K | 543.15 | Joback Method |
| cpg | 383.55 | J/mol×K | 578.92 | Joback Method |
| cpg | 398.95 | J/mol×K | 614.70 | Joback Method |
| cpg | 413.40 | J/mol×K | 650.48 | Joback Method |
| dvisc | 0.0001852 | Pa×s | 507.37 | Joback Method |
| dvisc | 0.0002397 | Pa×s | 469.29 | Joback Method |
| dvisc | 0.0025008 | Pa×s | 278.88 | Joback Method |
| dvisc | 0.0012488 | Pa×s | 316.96 | Joback Method |
| dvisc | 0.0007238 | Pa×s | 355.04 | Joback Method |
| dvisc | 0.0004663 | Pa×s | 393.12 | Joback Method |
| dvisc | 0.0003246 | Pa×s | 431.21 | Joback Method |
| hvapt | 59.80 | kJ/mol | 348.00 | NIST Webbook |
| hvapt | 56.50 ± 0.60 | kJ/mol | 301.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47383e+01 |
| Coeff. B | -4.10383e+03 |
| Coeff. C | -7.46320e+01 |
| Temperature range (K), min. | 358.62 |
| Temperature range (K), max. | 509.97 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C98191&Units=SI |
| **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/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **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 |

| | |
|---|---|
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |