# Benzene, 1-methyl-4-butyl

**Other names:** Benzene, 1-butyl-4-methyl-
1-Butyl-4-methylbenzene
1-Methyl-4-n-butylbenzene
**Inchi:** InChI=1S/C11H16/c1-3-4-5-11-8-6-10(2)7-9-11/h6-9H,3-5H2,1-2H3
**InchiKey:** SBBKUBSYOVDBBC-UHFFFAOYSA-N
**Formula:** C11H16
**SMILES:** CCCCc1ccc(C)cc1
**Mol. weight [g/mol]:** 148.24
**CAS:** 1595-05-7

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 144.52 | kJ/mol | Joback Method |
| hf | -45.31 | kJ/mol | Joback Method |
| hfus | 17.90 | kJ/mol | Joback Method |
| hvap | 43.02 | kJ/mol | Joback Method |
| ie | 8.40 ± 0.10 | eV | NIST Webbook |
| log10ws | -3.59 | | Crippen Method |
| logp | 3.338 | | Crippen Method |
| mcvol | 142.090 | ml/mol | McGowan Method |
| pc | 2608.40 | kPa | Joback Method |
| rinpol | 1146.00 | | NIST Webbook |
| rinpol | 1146.00 | | NIST Webbook |
| rinpol | 1139.00 | | NIST Webbook |
| rinpol | 1146.00 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1158.00 | | NIST Webbook |
| rinpol | 1146.10 | | NIST Webbook |
| rinpol | 1151.60 | | NIST Webbook |
| rinpol | 1158.10 | | NIST Webbook |
| rinpol | 1139.00 | | NIST Webbook |
| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1146.10 | | NIST Webbook |
| rinpol | 1146.00 | | NIST Webbook |
| rinpol | 1147.00 | | NIST Webbook |
| rinpol | 1152.00 | | NIST Webbook |
| rinpol | 1153.00 | | NIST Webbook |

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|---|---|---|---|
| rinpol | 1146.00 | | NIST Webbook |
| rinpol | 1146.00 | | NIST Webbook |
| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1135.00 | | NIST Webbook |
| ripol | 1391.60 | | NIST Webbook |
| ripol | 1375.00 | | NIST Webbook |
| ripol | 1375.00 | | NIST Webbook |
| ripol | 1375.30 | | NIST Webbook |
| tb | 471.00 ± 5.00 | K | NIST Webbook |
| tb | 471.65 ± 3.00 | K | NIST Webbook |
| tb | 480.20 | K | NIST Webbook |
| tb | 472.00 ± 5.00 | K | NIST Webbook |
| tc | 685.93 | K | Joback Method |
| tf | 188.00 ± 3.00 | K | NIST Webbook |
| vc | 0.543 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 300.77 | J/mol×K | 482.74 | Joback Method |
| cpg | 316.42 | J/mol×K | 516.60 | Joback Method |
| cpg | 331.27 | J/mol×K | 550.47 | Joback Method |
| cpg | 345.33 | J/mol×K | 584.33 | Joback Method |
| cpg | 358.64 | J/mol×K | 618.20 | Joback Method |
| cpg | 371.23 | J/mol×K | 652.06 | Joback Method |
| cpg | 383.12 | J/mol×K | 685.93 | Joback Method |
| dvisc | 0.0025675 | Pa×s | 252.67 | Joback Method |
| dvisc | 0.0012843 | Pa×s | 291.01 | Joback Method |
| dvisc | 0.0007549 | Pa×s | 329.36 | Joback Method |
| dvisc | 0.0004957 | Pa×s | 367.71 | Joback Method |
| dvisc | 0.0003524 | Pa×s | 406.05 | Joback Method |
| dvisc | 0.0002657 | Pa×s | 444.39 | Joback Method |
| dvisc | 0.0002096 | Pa×s | 482.74 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1595057&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

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|---|---|
| **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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical 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 |