# Benzene, (1-butylhexyl)-

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|---|---|
| **Other names:** | Decane, 5-phenyl-<br>(5-Decyl)benzene |
| **Inchi:** | InChI=1S/C16H26/c1-3-5-8-12-15(11-6-4-2)16-13-9-7-10-14-16/h7,9-10,13-15H,3-6,8,11 |
| **InchiKey:** | CDOBABYRHNVZQG-UHFFFAOYSA-N |
| **Formula:** | C16H26 |
| **SMILES:** | CCCCCC(CCCC)c1ccccc1 |
| **Mol. weight [g/mol]:** | 218.38 |
| **CAS:** | 4537-11-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 193.81 | kJ/mol | Joback Method |
| hf | -142.32 | kJ/mol | Joback Method |
| hfus | 27.71 | kJ/mol | Joback Method |
| hvap | 53.10 | kJ/mol | Joback Method |
| log10ws | -5.59 | | Crippen Method |
| logp | 5.541 | | Crippen Method |
| mcvol | 212.540 | ml/mol | McGowan Method |
| pc | 1714.61 | kPa | Joback Method |
| rinpol | 1535.00 | | NIST Webbook |
| rinpol | 263.10 | | NIST Webbook |
| rinpol | 1526.00 | | NIST Webbook |
| rinpol | 1537.00 | | NIST Webbook |
| rinpol | 1528.00 | | NIST Webbook |
| rinpol | 1526.00 | | NIST Webbook |
| ripol | 1729.00 | | NIST Webbook |
| ripol | 1729.00 | | NIST Webbook |
| tb | 591.72 | K | Joback Method |
| tc | 784.61 | K | Joback Method |
| tf | 281.50 | K | Joback Method |
| vc | 0.818 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 545.09 | J/mol×K | 591.72 | Joback Method |
| cpg | 564.58 | J/mol×K | 623.87 | Joback Method |
| cpg | 583.04 | J/mol×K | 656.02 | Joback Method |
| cpg | 600.51 | J/mol×K | 688.17 | Joback Method |
| cpg | 617.03 | J/mol×K | 720.31 | Joback Method |
| cpg | 632.64 | J/mol×K | 752.46 | Joback Method |
| cpg | 647.38 | J/mol×K | 784.61 | Joback Method |
| dvisc | 0.0047483 | Pa×s | 281.50 | Joback Method |
| dvisc | 0.0016769 | Pa×s | 333.20 | Joback Method |
| dvisc | 0.0007833 | Pa×s | 384.91 | Joback Method |
| dvisc | 0.0004381 | Pa×s | 436.61 | Joback Method |
| dvisc | 0.0002772 | Pa×s | 488.31 | Joback Method |
| dvisc | 0.0001914 | Pa×s | 540.02 | Joback Method |
| dvisc | 0.0001410 | Pa×s | 591.72 | Joback Method |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C4537115&Units=SI

# 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
**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 |