# 1-(2-Pentyl)-4-(3-pentyl)benzene

**Inchi:** InChI=1S/C16H26/c1-5-8-13(4)15-9-11-16(12-10-15)14(6-2)7-3/h9-14H,5-8H2,1-4H3
**InchiKey:** ZMJKPBLBOSIOHA-UHFFFAOYSA-N
**Formula:** C16H26
**SMILES:** CCCC(C)c1ccc(C(CC)CC)cc1
**Mol. weight [g/mol]:** 218.38
**CAS:** 101371-20-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 181.74 | kJ/mol | Joback Method |
| hf | -159.07 | kJ/mol | Joback Method |
| hfus | 23.80 | kJ/mol | Joback Method |
| hvap | 53.37 | kJ/mol | Joback Method |
| log10ws | -5.52 | | Crippen Method |
| logp | 5.494 | | Crippen Method |
| mcvol | 212.540 | ml/mol | McGowan Method |
| pc | 1704.71 | kPa | Joback Method |
| tb | 596.26 | K | Joback Method |
| tc | 793.83 | K | Joback Method |
| tf | 279.02 | K | Joback Method |
| vc | 0.811 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 545.90 | J/mol×K | 596.26 | Joback Method |
| cpg | 634.22 | J/mol×K | 760.90 | Joback Method |
| cpg | 618.49 | J/mol×K | 727.97 | Joback Method |
| cpg | 601.82 | J/mol×K | 695.05 | Joback Method |
| cpg | 584.20 | J/mol×K | 662.12 | Joback Method |
| cpg | 565.57 | J/mol×K | 629.19 | Joback Method |
| cpg | 649.07 | J/mol×K | 793.83 | Joback Method |
| dvisc | 0.0001293 | Pa×s | 596.26 | Joback Method |
| dvisc | 0.0001756 | Pa×s | 543.39 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002546 | Pa×s | 490.51 | Joback Method |
| dvisc | 0.0004041 | Pa×s | 437.64 | Joback Method |
| dvisc | 0.0007280 | Pa×s | 384.77 | Joback Method |
| dvisc | 0.0015822 | Pa×s | 331.89 | Joback Method |
| dvisc | 0.0046147 | Pa×s | 279.02 | 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=C101371204&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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume