# 4,5-diphenyl-1,3-hexadiene

**Inchi:** InChI=1S/C18H18/c1-3-10-18(17-13-8-5-9-14-17)15(2)16-11-6-4-7-12-16/h3-15H,1H2,2H
**InchiKey:** CCPVGOJXSGZKOT-ZDLGFXPLSA-N
**Formula:** C18H18
**SMILES:** C=CC=C(c1ccccc1)C(C)c1ccccc1
**Mol. weight [g/mol]:** 234.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 482.57 | kJ/mol | Joback Method |
| hf | 285.79 | kJ/mol | Joback Method |
| hfus | 24.55 | kJ/mol | Joback Method |
| hvap | 59.19 | kJ/mol | Joback Method |
| log10ws | -5.40 | | Crippen Method |
| logp | 5.060 | | Crippen Method |
| mcvol | 208.360 | ml/mol | McGowan Method |
| pc | 2110.00 | kPa | Joback Method |
| rinpol | 1874.40 | | NIST Webbook |
| rinpol | 1874.40 | | NIST Webbook |
| tb | 664.88 | K | Joback Method |
| tc | 909.31 | K | Joback Method |
| tf | 309.66 | K | Joback Method |
| vc | 0.783 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 533.14 | J/mol×K | 664.88 | Joback Method |
| cpg | 552.05 | J/mol×K | 705.62 | Joback Method |
| cpg | 569.46 | J/mol×K | 746.36 | Joback Method |
| cpg | 585.50 | J/mol×K | 787.10 | Joback Method |
| cpg | 600.30 | J/mol×K | 827.83 | Joback Method |
| cpg | 613.98 | J/mol×K | 868.57 | Joback Method |
| cpg | 626.68 | J/mol×K | 909.31 | 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=R316386&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |