# 1,4-diphenyl-2-penten-2-one

**Inchi:** InChI=1S/C17H16O/c1-14(16-10-6-3-7-11-16)12-17(18)13-15-8-4-2-5-9-15/h2-12H,13H2
**InchiKey:** PKMNPZTZDALEFS-WYMLVPIESA-N
**Formula:** C17H16O
**SMILES:** CC(=CC(=O)Cc1ccccc1)c1ccccc1
**Mol. weight [g/mol]:** 236.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 259.83 | kJ/mol | Joback Method |
| hf | 73.70 | kJ/mol | Joback Method |
| hfus | 28.36 | kJ/mol | Joback Method |
| hvap | 64.77 | kJ/mol | Joback Method |
| log10ws | -4.45 | | Crippen Method |
| logp | 3.902 | | Crippen Method |
| mcvol | 200.140 | ml/mol | McGowan Method |
| pc | 2338.29 | kPa | Joback Method |
| rinpol | 2010.60 | | NIST Webbook |
| tb | 699.63 | K | Joback Method |
| tc | 944.85 | K | Joback Method |
| tf | 365.08 | K | Joback Method |
| vc | 0.758 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 521.72 | J/mol×K | 699.63 | Joback Method |
| cpg | 538.38 | J/mol×K | 740.50 | Joback Method |
| cpg | 553.69 | J/mol×K | 781.37 | Joback Method |
| cpg | 567.77 | J/mol×K | 822.24 | Joback Method |
| cpg | 580.73 | J/mol×K | 863.11 | Joback Method |
| cpg | 592.68 | J/mol×K | 903.98 | Joback Method |
| cpg | 603.75 | J/mol×K | 944.85 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R316237&Units=SI |
| **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 |
| **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 |

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