# 2,2-Dimethyl-1,3-diphenyl-1,3-propanedione

**Other names:** 2,2-Dimethyl-1,3-diphenyl-1,3-propanedione
**Inchi:** InChI=1S/C17H16O2/c1-17(2,15(18)13-9-5-3-6-10-13)16(19)14-11-7-4-8-12-14/h3-12H,1
**InchiKey:** ZCQWHDYGRXASIN-UHFFFAOYSA-N
**Formula:** C17H16O2
**SMILES:** CC(C)(C(=O)c1ccccc1)C(=O)c1ccccc1
**Mol. weight [g/mol]:** 252.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5317 | | Cheméo Relay (1.0) |
| gf | 62.08 | kJ/mol | Joback Method |
| hf | -154.82 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 23.65 | kJ/mol | Joback Method |
| hvap | 87.15 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.00 ± 0.05 | eV | NIST Webbook |
| log10ws | -4.32 | | Cheméo Relay (1.0) |
| logp | 3.778 | | Crippen Method |
| mcvol | 206.010 | ml/mol | McGowan Method |
| pc | 2395.87 | kPa | Joback Method |
| tb | 601.60 | K | Cheméo Relay (1.0) |
| tc | 876.83 | K | Cheméo Relay (1.0) |
| tf | 372.96 | K | Cheméo Relay (1.0) |
| vc | 0.745 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 563.88 | J/mol×K | 746.23 | Joback Method |
| cpg | 579.29 | J/mol×K | 787.98 | Joback Method |
| cpg | 593.31 | J/mol×K | 829.73 | Joback Method |
| cpg | 606.07 | J/mol×K | 871.48 | Joback Method |
| cpg | 617.70 | J/mol×K | 913.22 | Joback Method |
| cpg | 628.34 | J/mol×K | 954.97 | Joback Method |
| cpg | 638.10 | J/mol×K | 996.72 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0015226 | Pa×s | 436.47 | Joback Method |
| dvisc | 0.0007894 | Pa×s | 488.10 | Joback Method |
| dvisc | 0.0004640 | Pa×s | 539.72 | Joback Method |
| dvisc | 0.0002993 | Pa×s | 591.35 | Joback Method |
| dvisc | 0.0002071 | Pa×s | 642.98 | Joback Method |
| dvisc | 0.0001514 | Pa×s | 694.60 | Joback Method |
| dvisc | 0.0001156 | Pa×s | 746.23 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C41169420&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |