# Dimethyl phenylethyl carbinyl acetate

**Other names:** 1,1-dimethyl-3-phenylpropyl acetate
**Inchi:** InChI=1S/C13H18O2/c1-11(14)15-13(2,3)10-9-12-7-5-4-6-8-12/h4-8H,9-10H2,1-3H3
**InchiKey:** ZXFNOEJFYLQUSB-UHFFFAOYSA-N
**Formula:** C13H18O2
**SMILES:** CC(=O)OC(C)(C)CCc1ccccc1
**Mol. weight [g/mol]:** 206.28
**CAS:** 103-07-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -60.09 | kJ/mol | Joback Method |
| hf | -328.67 | kJ/mol | Joback Method |
| hfus | 18.84 | kJ/mol | Joback Method |
| hvap | 54.67 | kJ/mol | Joback Method |
| log10ws | -3.34 | | Crippen Method |
| logp | 2.961 | | Crippen Method |
| mcvol | 177.710 | ml/mol | McGowan Method |
| pc | 2333.78 | kPa | Joback Method |
| rinpol | 1424.00 | | NIST Webbook |
| rinpol | 1423.70 | | NIST Webbook |
| tb | 596.58 | K | Joback Method |
| tc | 811.41 | K | Joback Method |
| tf | 337.27 | K | Joback Method |
| vc | 0.668 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 446.48 | J/mol×K | 596.58 | Joback Method |
| cpg | 463.14 | J/mol×K | 632.38 | Joback Method |
| cpg | 478.72 | J/mol×K | 668.19 | Joback Method |
| cpg | 493.27 | J/mol×K | 703.99 | Joback Method |
| cpg | 506.83 | J/mol×K | 739.80 | Joback Method |
| cpg | 519.47 | J/mol×K | 775.60 | Joback Method |

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|---|---|---|---|---|
| cpg | 531.22 | J/mol×K | 811.41 | Joback Method |
| dvisc | 0.0024771 | Pa×s | 337.27 | Joback Method |
| dvisc | 0.0011900 | Pa×s | 380.49 | Joback Method |
| dvisc | 0.0006639 | Pa×s | 423.71 | Joback Method |
| dvisc | 0.0004127 | Pa×s | 466.92 | Joback Method |
| dvisc | 0.0002780 | Pa×s | 510.14 | Joback Method |
| dvisc | 0.0001992 | Pa×s | 553.36 | Joback Method |
| dvisc | 0.0001498 | Pa×s | 596.58 | Joback Method |

# Sources

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|---|---|
| **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=C103071&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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