# Citronellyl benzoate

**Other names:** 3,7-Dimethyloct-6-en-1-yl benzoate
**Inchi:** InChI=1S/C17H24O2/c1-14(2)8-7-9-15(3)12-13-19-17(18)16-10-5-4-6-11-16/h4-6,8,10-1
**InchiKey:** UDPCCAUIDDVTEL-UHFFFAOYSA-N
**Formula:** C17H24O2
**SMILES:** CC(C)=CCCC(C)CCOC(=O)c1ccccc1
**Mol. weight [g/mol]:** 260.37
**CAS:** 10482-77-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 39.98 | kJ/mol | Joback Method |
| hf | -300.33 | kJ/mol | Joback Method |
| hfus | 31.98 | kJ/mol | Joback Method |
| hvap | 64.52 | kJ/mol | Joback Method |
| log10ws | -5.09 | | Crippen Method |
| logp | 4.616 | | Crippen Method |
| mcvol | 229.770 | ml/mol | McGowan Method |
| pc | 1724.59 | kPa | Joback Method |
| rinpol | 1929.70 | | NIST Webbook |
| rinpol | 1929.70 | | NIST Webbook |
| ripol | 2512.00 | | NIST Webbook |
| ripol | 2512.00 | | NIST Webbook |
| tb | 694.93 | K | Joback Method |
| tc | 901.07 | K | Joback Method |
| tf | 345.89 | K | Joback Method |
| vc | 0.878 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 632.49 | J/mol×K | 694.93 | Joback Method |
| cpg | 650.04 | J/mol×K | 729.29 | Joback Method |
| cpg | 666.53 | J/mol×K | 763.64 | Joback Method |
| cpg | 682.01 | J/mol×K | 798.00 | Joback Method |

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|---|---|---|---|---|
| cpg | 696.52 | J/mol×K | 832.36 | Joback Method |
| cpg | 710.11 | J/mol×K | 866.72 | Joback Method |
| cpg | 722.83 | J/mol×K | 901.07 | Joback Method |

# Sources

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|---|---|
| **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=C10482776&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |