# Benzyl angelate

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|---|---|
| **Inchi:** | InChI=1S/C12H14O2/c1-3-10(2)12(13)14-9-11-7-5-4-6-8-11/h3-8H,9H2,1-2H3/b10-3- |
| **InchiKey:** | QRGSTISKDZCDHV-KMKOMSMNSA-N |
| **Formula:** | C12H14O2 |
| **SMILES:** | CC=C(C)C(=O)OCc1ccccc1 |
| **Mol. weight [g/mol]:** | 190.24 |
| **CAS:** | 37526-87-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 0.32 | kJ/mol | Joback Method |
| hf | -191.85 | kJ/mol | Joback Method |
| hfus | 22.56 | kJ/mol | Joback Method |
| hvap | 53.78 | kJ/mol | Joback Method |
| log10ws | -3.16 | | Crippen Method |
| logp | 2.696 | | Crippen Method |
| mcvol | 159.320 | ml/mol | McGowan Method |
| pc | 2668.02 | kPa | Joback Method |
| rinpol | 1446.40 | | NIST Webbook |
| rinpol | 1446.40 | | NIST Webbook |
| tb | 580.97 | K | Joback Method |
| tc | 799.81 | K | Joback Method |
| tf | 304.54 | K | Joback Method |
| vc | 0.605 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 374.15 | J/mol×K | 580.97 | Joback Method |
| cpg | 389.04 | J/mol×K | 617.44 | Joback Method |
| cpg | 402.99 | J/mol×K | 653.92 | Joback Method |
| cpg | 416.04 | J/mol×K | 690.39 | Joback Method |
| cpg | 428.24 | J/mol×K | 726.86 | Joback Method |
| cpg | 439.62 | J/mol×K | 763.34 | Joback Method |
| cpg | 450.23 | J/mol×K | 799.81 | 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=C37526877&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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