# Avenaciolide, 6-(2-phenylethyl)-4-demethylene

**Inchi:** InChI=1S/C14H14O4/c15-12-8-10-11(17-14(16)13(10)18-12)7-6-9-4-2-1-3-5-9/h1-5,10-1
**InchiKey:** JPDNKTJUDXVCLT-NQBHXWOUSA-N
**Formula:** C14H14O4
**SMILES:** O=C1CC2C(CCc3ccccc3)OC(=O)C2O1
**Mol. weight [g/mol]:** 246.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -148.42 | kJ/mol | Joback Method |
| hf | -522.22 | kJ/mol | Joback Method |
| hfus | 34.18 | kJ/mol | Joback Method |
| hvap | 66.41 | kJ/mol | Joback Method |
| log10ws | -2.28 | | Crippen Method |
| logp | 1.476 | | Crippen Method |
| mcvol | 177.520 | ml/mol | McGowan Method |
| pc | 2764.26 | kPa | Joback Method |
| rinpol | 2207.00 | | NIST Webbook |
| rinpol | 2207.00 | | NIST Webbook |
| tb | 753.29 | K | Joback Method |
| tc | 1009.99 | K | Joback Method |
| tf | 488.14 | K | Joback Method |
| vc | 0.664 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 550.19 | J/mol×K | 753.29 | Joback Method |
| cpg | 567.73 | J/mol×K | 796.07 | Joback Method |
| cpg | 583.70 | J/mol×K | 838.86 | Joback Method |
| cpg | 598.11 | J/mol×K | 881.64 | Joback Method |
| cpg | 610.99 | J/mol×K | 924.42 | Joback Method |
| cpg | 622.36 | J/mol×K | 967.21 | Joback Method |
| cpg | 632.25 | J/mol×K | 1009.99 | 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=R565890&Units=SI |

# 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 |