# Avenaciolide, 1-dihydro-6-[2-(4-trifluoromethylphenyl)ethyl]-4-d

**Inchi:** InChI=1S/C15H15F3O4/c16-15(17,18)11-4-1-10(2-5-11)3-6-12-7-8-13(19)21-9-14(20)22

**InchiKey:** NHMLMBUQUDCMEZ-GFCCVEGCSA-N

**Formula:** C15H15F3O4

**SMILES:** O=C1CCC(CCc2ccc(C(F)(F)F)cc2)OC(=O)CO1

**Mol. weight [g/mol]:** 316.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -820.56 | kJ/mol | Joback Method |
| hf | -1222.35 | kJ/mol | Joback Method |
| hfus | 32.70 | kJ/mol | Joback Method |
| hvap | 66.46 | kJ/mol | Joback Method |
| log10ws | -3.62 | | Crippen Method |
| logp | 2.887 | | Crippen Method |
| mcvol | 207.780 | ml/mol | McGowan Method |
| pc | 2161.32 | kPa | Joback Method |
| rinpol | 2175.00 | | NIST Webbook |
| rinpol | 2175.00 | | NIST Webbook |
| tb | 786.47 | K | Joback Method |
| tc | 1026.30 | K | Joback Method |
| tf | 491.86 | K | Joback Method |
| vc | 0.783 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 652.03 | J/mol×K | 786.47 | Joback Method |
| cpg | 668.59 | J/mol×K | 826.44 | Joback Method |
| cpg | 683.42 | J/mol×K | 866.41 | Joback Method |
| cpg | 696.51 | J/mol×K | 906.38 | Joback Method |
| cpg | 707.83 | J/mol×K | 946.36 | Joback Method |
| cpg | 717.38 | J/mol×K | 986.33 | Joback Method |
| cpg | 725.15 | J/mol×K | 1026.30 | 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=R565701&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 |