# 1-(3,4-Dimethoxyphenyl)pentan-3-one

**Inchi:** InChI=1S/C13H18O3/c1-4-11(14)7-5-10-6-8-12(15-2)13(9-10)16-3/h6,8-9H,4-5,7H2,1-3H
**InchiKey:** SOWKMIKWOOVRAB-UHFFFAOYSA-N
**Formula:** C13H18O3
**SMILES:** CCC(=O)CCc1ccc(OC)c(OC)c1
**Mol. weight [g/mol]:** 222.28
**CAS:** 39728-56-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -187.19 | kJ/mol | Joback Method |
| hf | -475.08 | kJ/mol | Joback Method |
| hfus | 26.66 | kJ/mol | Joback Method |
| hvap | 59.70 | kJ/mol | Joback Method |
| log10ws | -3.05 | | Crippen Method |
| logp | 2.615 | | Crippen Method |
| mcvol | 183.580 | ml/mol | McGowan Method |
| pc | 2191.78 | kPa | Joback Method |
| rinpol | 1786.50 | | NIST Webbook |
| rinpol | 1786.50 | | NIST Webbook |
| tb | 632.19 | K | Joback Method |
| tc | 835.04 | K | Joback Method |
| tf | 382.12 | K | Joback Method |
| vc | 0.698 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 468.92 | J/mol×K | 632.19 | Joback Method |
| cpg | 484.01 | J/mol×K | 666.00 | Joback Method |
| cpg | 498.32 | J/mol×K | 699.81 | Joback Method |
| cpg | 511.85 | J/mol×K | 733.62 | Joback Method |
| cpg | 524.61 | J/mol×K | 767.43 | Joback Method |
| cpg | 536.60 | J/mol×K | 801.23 | Joback Method |
| cpg | 547.81 | J/mol×K | 835.04 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0009821 | Pa×s | 382.12 | Joback Method |
| dvisc | 0.0005937 | Pa×s | 423.80 | Joback Method |
| dvisc | 0.0003927 | Pa×s | 465.48 | Joback Method |
| dvisc | 0.0002781 | Pa×s | 507.16 | Joback Method |
| dvisc | 0.0002075 | Pa×s | 548.83 | Joback Method |
| dvisc | 0.0001613 | Pa×s | 590.51 | Joback Method |
| dvisc | 0.0001297 | Pa×s | 632.19 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C39728568&Units=SI |
| **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 |

# 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 |