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

**Inchi:** InChI=1S/C14H20O3/c1-4-5-12(15)8-6-11-7-9-13(16-2)14(10-11)17-3/h7,9-10H,4-6,8H2,
**InchiKey:** PQRJLNAKELCEAC-UHFFFAOYSA-N
**Formula:** C14H20O3
**SMILES:** CCCC(=O)CCc1ccc(OC)c(OC)c1
**Mol. weight [g/mol]:** 236.31
**CAS:** 39728-57-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -178.77 | kJ/mol | Joback Method |
| hf | -495.72 | kJ/mol | Joback Method |
| hfus | 29.25 | kJ/mol | Joback Method |
| hvap | 61.92 | kJ/mol | Joback Method |
| log10ws | -3.47 | | Crippen Method |
| logp | 3.006 | | Crippen Method |
| mcvol | 197.670 | ml/mol | McGowan Method |
| pc | 2007.30 | kPa | Joback Method |
| rinpol | 1828.50 | | NIST Webbook |
| rinpol | 1828.50 | | NIST Webbook |
| tb | 655.07 | K | Joback Method |
| tc | 855.23 | K | Joback Method |
| tf | 393.39 | K | Joback Method |
| vc | 0.753 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 520.54 | J/mol×K | 655.07 | Joback Method |
| cpg | 590.56 | J/mol×K | 821.87 | Joback Method |
| cpg | 578.19 | J/mol×K | 788.51 | Joback Method |
| cpg | 565.00 | J/mol×K | 755.15 | Joback Method |
| cpg | 551.00 | J/mol×K | 721.79 | Joback Method |
| cpg | 536.18 | J/mol×K | 688.43 | Joback Method |
| cpg | 602.13 | J/mol×K | 855.23 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001171 | Pa×s | 655.07 | Joback Method |
| dvisc | 0.0001464 | Pa×s | 611.46 | Joback Method |
| dvisc | 0.0001894 | Pa×s | 567.84 | Joback Method |
| dvisc | 0.0002557 | Pa×s | 524.23 | Joback Method |
| dvisc | 0.0003646 | Pa×s | 480.62 | Joback Method |
| dvisc | 0.0005581 | Pa×s | 437.00 | Joback Method |
| dvisc | 0.0009388 | Pa×s | 393.39 | Joback Method |

# Sources

| | |
|---|---|
| **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=C39728579&Units=SI |

# 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 |