# 2-Propenoic acid, 3-(3,4-dimethoxyphenyl)-, methyl ester, cis

**Inchi:** InChI=1S/C13H16O5/c1-15-10-7-9(5-6-12(14)17-3)8-11(16-2)13(10)18-4/h5-8H,1-4H3/b

**InchiKey:** KLXHCGFNNUQTEY-WAYWQWQTSA-N

**Formula:** C13H16O5

**SMILES:** COC(=O)C=Cc1cc(OC)c(OC)c(OC)c1

**Mol. weight [g/mol]:** 252.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -326.60 | kJ/mol | Joback Method |
| hf | -633.77 | kJ/mol | Joback Method |
| hfus | 28.85 | kJ/mol | Joback Method |
| hvap | 65.14 | kJ/mol | Joback Method |
| log10ws | -2.35 | | Crippen Method |
| logp | 1.899 | | Crippen Method |
| mcvol | 191.020 | ml/mol | McGowan Method |
| pc | 2197.95 | kPa | Joback Method |
| rinpol | 1730.00 | | NIST Webbook |
| tb | 686.17 | K | Joback Method |
| tc | 893.75 | K | Joback Method |
| tf | 434.02 | K | Joback Method |
| vc | 0.714 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 498.43 | J/mol×K | 686.17 | Joback Method |
| cpg | 560.19 | J/mol×K | 859.15 | Joback Method |
| cpg | 549.47 | J/mol×K | 824.56 | Joback Method |
| cpg | 537.90 | J/mol×K | 789.96 | Joback Method |
| cpg | 525.53 | J/mol×K | 755.36 | Joback Method |
| cpg | 512.36 | J/mol×K | 720.77 | Joback Method |
| cpg | 570.06 | J/mol×K | 893.75 | Joback Method |
| dvisc | 0.0000688 | Pa×s | 686.17 | Joback Method |
| dvisc | 0.0000842 | Pa×s | 644.15 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001060 | Pa×s | 602.12 | Joback Method |
| dvisc | 0.0001381 | Pa×s | 560.10 | Joback Method |
| dvisc | 0.0001879 | Pa×s | 518.07 | Joback Method |
| dvisc | 0.0002698 | Pa×s | 476.05 | Joback Method |
| dvisc | 0.0004157 | Pa×s | 434.02 | Joback Method |

# Sources

| | |
|---|---|
| **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=R298456&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |