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

**Inchi:** InChI=1S/C12H14O4/c1-14-10-6-4-9(8-11(10)15-2)5-7-12(13)16-3/h4-8H,1-3H3/b7-5+

**InchiKey:** JXRYDOZRPYFBKO-FNORWQNLSA-N

**Formula:** C12H14O4

**SMILES:** COC(=O)C=Cc1ccc(OC)c(OC)c1

**Mol. weight [g/mol]:** 222.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -220.39 | kJ/mol | Joback Method |
| hf | -469.44 | kJ/mol | Joback Method |
| hfus | 25.46 | kJ/mol | Joback Method |
| hvap | 59.84 | kJ/mol | Joback Method |
| log10ws | -2.23 | | Crippen Method |
| logp | 1.890 | | Crippen Method |
| mcvol | 171.060 | ml/mol | McGowan Method |
| pc | 2487.55 | kPa | Joback Method |
| rinpol | 1835.00 | | NIST Webbook |
| tb | 635.89 | K | Joback Method |
| tc | 847.87 | K | Joback Method |
| tf | 388.00 | K | Joback Method |
| vc | 0.639 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 422.99 | J/mol×K | 635.89 | Joback Method |
| cpg | 483.89 | J/mol×K | 812.54 | Joback Method |
| cpg | 473.21 | J/mol×K | 777.21 | Joback Method |
| cpg | 461.77 | J/mol×K | 741.88 | Joback Method |
| cpg | 449.59 | J/mol×K | 706.55 | Joback Method |
| cpg | 436.66 | J/mol×K | 671.22 | Joback Method |
| cpg | 493.81 | J/mol×K | 847.87 | Joback Method |
| dvisc | 0.0000976 | Pa×s | 635.89 | Joback Method |
| dvisc | 0.0001209 | Pa×s | 594.58 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001546 | Pa×s | 553.26 | Joback Method |
| dvisc | 0.0002058 | Pa×s | 511.94 | Joback Method |
| dvisc | 0.0002880 | Pa×s | 470.63 | Joback Method |
| dvisc | 0.0004299 | Pa×s | 429.31 | Joback Method |
| dvisc | 0.0006990 | Pa×s | 388.00 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R298421&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

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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