# Fumaric acid, 3,4-dimethoxyphenyl tridecyl ester

**Inchi:** InChI=1S/C25H38O6/c1-4-5-6-7-8-9-10-11-12-13-14-19-30-24(26)17-18-25(27)31-21-15
**InchiKey:** WLOVWAUMUNMRJE-ISLYRVAYSA-N
**Formula:** C25H38O6
**SMILES:** CCCCCCCCCCCCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1
**Mol. weight [g/mol]:** 434.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -344.85 | kJ/mol | Joback Method |
| hf | -982.56 | kJ/mol | Joback Method |
| hfus | 61.92 | kJ/mol | Joback Method |
| hvap | 97.93 | kJ/mol | Joback Method |
| log10ws | -7.02 | | Crippen Method |
| logp | 6.020 | | Crippen Method |
| mcvol | 361.670 | ml/mol | McGowan Method |
| pc | 972.30 | kPa | Joback Method |
| rinpol | 3304.00 | | NIST Webbook |
| rinpol | 3304.00 | | NIST Webbook |
| tb | 1009.62 | K | Joback Method |
| tc | 1236.87 | K | Joback Method |
| tf | 606.67 | K | Joback Method |
| vc | 1.391 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1210.10 | J/mol×K | 1009.62 | Joback Method |
| cpg | 1225.32 | J/mol×K | 1047.49 | Joback Method |
| cpg | 1238.80 | J/mol×K | 1085.37 | Joback Method |
| cpg | 1250.55 | J/mol×K | 1123.24 | Joback Method |
| cpg | 1260.60 | J/mol×K | 1161.12 | Joback Method |
| cpg | 1268.97 | J/mol×K | 1198.99 | Joback Method |
| cpg | 1275.69 | J/mol×K | 1236.87 | Joback Method |
| dvisc | 0.0001343 | Pa×s | 606.67 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000749 | Pa×s | 673.83 | Joback Method |
| dvisc | 0.0000465 | Pa×s | 740.99 | Joback Method |
| dvisc | 0.0000312 | Pa×s | 808.14 | Joback Method |
| dvisc | 0.0000223 | Pa×s | 875.30 | Joback Method |
| dvisc | 0.0000167 | Pa×s | 942.46 | Joback Method |
| dvisc | 0.0000130 | Pa×s | 1009.62 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348175&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

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|---|---|
| **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 |