# Fumaric acid, 2,6-dimethoxyphenyl 3-chlorophenyl ester

**Inchi:** InChI=1S/C18H15ClO6/c1-22-14-7-4-8-15(23-2)18(14)25-17(21)10-9-16(20)24-13-6-3-5-

**InchiKey:** WFSYBIHBIQZNBT-MDZDMXLPSA-N

**Formula:** C18H15ClO6

**SMILES:** COc1cccc(OC)c1OC(=O)C=CC(=O)Oc1cccc(Cl)c1

**Mol. weight [g/mol]:** 362.76

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -312.94 | kJ/mol | Joback Method |
| hf | -628.76 | kJ/mol | Joback Method |
| hfus | 41.64 | kJ/mol | Joback Method |
| hvap | 89.67 | kJ/mol | Joback Method |
| log10ws | -4.53 | | Crippen Method |
| logp | 3.424 | | Crippen Method |
| mcvol | 251.520 | ml/mol | McGowan Method |
| pc | 1964.82 | kPa | Joback Method |
| rinpol | 2730.00 | | NIST Webbook |
| rinpol | 2730.00 | | NIST Webbook |
| tb | 918.55 | K | Joback Method |
| tc | 1154.65 | K | Joback Method |
| tf | 596.64 | K | Joback Method |
| vc | 0.941 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 711.32 | J/mol×K | 918.55 | Joback Method |
| cpg | 721.81 | J/mol×K | 957.90 | Joback Method |
| cpg | 730.93 | J/mol×K | 997.25 | Joback Method |
| cpg | 738.68 | J/mol×K | 1036.60 | Joback Method |
| cpg | 745.05 | J/mol×K | 1075.95 | Joback Method |
| cpg | 750.04 | J/mol×K | 1115.30 | Joback Method |
| cpg | 753.65 | J/mol×K | 1154.65 | Joback Method |
| dvisc | 0.0001963 | Pa×s | 596.64 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001288 | Pa×s | 650.29 | Joback Method |
| dvisc | 0.0000901 | Pa×s | 703.94 | Joback Method |
| dvisc | 0.0000663 | Pa×s | 757.60 | Joback Method |
| dvisc | 0.0000508 | Pa×s | 811.25 | Joback Method |
| dvisc | 0.0000403 | Pa×s | 864.90 | Joback Method |
| dvisc | 0.0000328 | Pa×s | 918.55 | 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=U405759&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