# Fumaric acid, 2-chlorophenyl 2,3-dichlorophenyl ester

**Inchi:** InChI=1S/C16H9Cl3O4/c17-10-4-1-2-6-12(10)22-14(20)8-9-15(21)23-13-7-3-5-11(18)16(
**InchiKey:** YDEGGRUWAGVFPN-CMDGGOBGSA-N
**Formula:** C16H9Cl3O4
**SMILES:** O=C(C=CC(=O)Oc1cccc(Cl)c1Cl)Oc1ccccc1Cl
**Mol. weight [g/mol]:** 371.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -143.64 | kJ/mol | Joback Method |
| hf | -354.52 | kJ/mol | Joback Method |
| hfus | 42.48 | kJ/mol | Joback Method |
| hvap | 89.17 | kJ/mol | Joback Method |
| log10ws | -5.66 | | Crippen Method |
| logp | 4.714 | | Crippen Method |
| mcvol | 236.080 | ml/mol | McGowan Method |
| pc | 2258.96 | kPa | Joback Method |
| rinpol | 2687.00 | | NIST Webbook |
| rinpol | 2687.00 | | NIST Webbook |
| tb | 902.81 | K | Joback Method |
| tc | 1154.56 | K | Joback Method |
| tf | 589.48 | K | Joback Method |
| vc | 0.890 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 589.02 | J/mol×K | 902.81 | Joback Method |
| cpg | 597.86 | J/mol×K | 944.77 | Joback Method |
| cpg | 605.64 | J/mol×K | 986.73 | Joback Method |
| cpg | 612.39 | J/mol×K | 1028.69 | Joback Method |
| cpg | 618.16 | J/mol×K | 1070.65 | Joback Method |
| cpg | 622.99 | J/mol×K | 1112.60 | Joback Method |
| cpg | 626.94 | J/mol×K | 1154.56 | Joback Method |
| dvisc | 0.0003288 | Pa×s | 589.48 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002186 | Pa×s | 641.70 | Joback Method |
| dvisc | 0.0001545 | Pa×s | 693.92 | Joback Method |
| dvisc | 0.0001147 | Pa×s | 746.14 | Joback Method |
| dvisc | 0.0000885 | Pa×s | 798.37 | Joback Method |
| dvisc | 0.0000705 | Pa×s | 850.59 | Joback Method |
| dvisc | 0.0000577 | Pa×s | 902.81 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405726&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 |