# Fumaric acid, 1-phenylprop-1-yl 2,2-dichloroethyl ester

**Inchi:** InChI=1S/C15H16Cl2O4/c1-2-12(11-6-4-3-5-7-11)21-15(19)9-8-14(18)20-10-13(16)17/h3

**InchiKey:** LJAZILGVFMIGHS-CMDGGOBGSA-N

**Formula:** C15H16Cl2O4

**SMILES:** CCC(OC(=O)C=CC(=O)OCC(Cl)Cl)c1ccccc1

**Mol. weight [g/mol]:** 331.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -228.53 | kJ/mol | Joback Method |
| hf | -530.82 | kJ/mol | Joback Method |
| hfus | 35.77 | kJ/mol | Joback Method |
| hvap | 77.52 | kJ/mol | Joback Method |
| log10ws | -4.16 | | Crippen Method |
| logp | 3.584 | | Crippen Method |
| mcvol | 233.510 | ml/mol | McGowan Method |
| pc | 1991.21 | kPa | Joback Method |
| rinpol | 2188.00 | | NIST Webbook |
| rinpol | 2188.00 | | NIST Webbook |
| tb | 800.00 | K | Joback Method |
| tc | 1022.79 | K | Joback Method |
| tf | 454.31 | K | Joback Method |
| vc | 0.881 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 621.15 | J/mol×K | 800.00 | Joback Method |
| cpg | 633.61 | J/mol×K | 837.13 | Joback Method |
| cpg | 645.05 | J/mol×K | 874.26 | Joback Method |
| cpg | 655.51 | J/mol×K | 911.40 | Joback Method |
| cpg | 665.03 | J/mol×K | 948.53 | Joback Method |
| cpg | 673.65 | J/mol×K | 985.66 | Joback Method |
| cpg | 681.40 | J/mol×K | 1022.79 | Joback Method |
| dvisc | 0.0009407 | Pa×s | 454.31 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004601 | Pa×s | 511.93 | Joback Method |
| dvisc | 0.0002600 | Pa×s | 569.54 | Joback Method |
| dvisc | 0.0001632 | Pa×s | 627.15 | Joback Method |
| dvisc | 0.0001108 | Pa×s | 684.77 | Joback Method |
| dvisc | 0.0000799 | Pa×s | 742.38 | Joback Method |
| dvisc | 0.0000604 | Pa×s | 800.00 | Joback Method |

# Sources

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|---|---|
| **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=U405899&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 |