# Fumaric acid, decyl 2,2,2-trichloroethyl ester

**Inchi:** InChI=1S/C16H25Cl3O4/c1-2-3-4-5-6-7-8-9-12-22-14(20)10-11-15(21)23-13-16(17,18)19
**InchiKey:** KZHVAYZESXTNDB-ZHACJKMWSA-N
**Formula:** C16H25Cl3O4
**SMILES:** CCCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl
**Mol. weight [g/mol]:** 387.73

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -336.73 | kJ/mol | Joback Method |
| hf | -801.92 | kJ/mol | Joback Method |
| hfus | 48.15 | kJ/mol | Joback Method |
| hvap | 81.34 | kJ/mol | Joback Method |
| log10ws | -5.66 | | Crippen Method |
| logp | 5.140 | | Crippen Method |
| mcvol | 283.600 | ml/mol | McGowan Method |
| pc | 1369.71 | kPa | Joback Method |
| rinpol | 2380.00 | | NIST Webbook |
| tb | 831.28 | K | Joback Method |
| tc | 1031.86 | K | Joback Method |
| tf | 501.50 | K | Joback Method |
| vc | 1.095 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 796.28 | J/mol×K | 831.28 | Joback Method |
| cpg | 855.06 | J/mol×K | 998.43 | Joback Method |
| cpg | 844.87 | J/mol×K | 965.00 | Joback Method |
| cpg | 833.95 | J/mol×K | 931.57 | Joback Method |
| cpg | 822.24 | J/mol×K | 898.14 | Joback Method |
| cpg | 809.70 | J/mol×K | 864.71 | Joback Method |
| cpg | 864.55 | J/mol×K | 1031.86 | Joback Method |
| dvisc | 0.0000415 | Pa×s | 831.28 | Joback Method |
| dvisc | 0.0000548 | Pa×s | 776.32 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000757 | Pa×s | 721.35 | Joback Method |
| dvisc | 0.0001102 | Pa×s | 666.39 | Joback Method |
| dvisc | 0.0001716 | Pa×s | 611.43 | Joback Method |
| dvisc | 0.0002918 | Pa×s | 556.46 | Joback Method |
| dvisc | 0.0005571 | Pa×s | 501.50 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348507&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 |