# Fumaric acid, pentafluorobenzyl 2,4,6-trichlorophenyl ester

**Inchi:** InChI=1S/C17H6Cl3F5O4/c18-6-3-8(19)17(9(20)4-6)29-11(27)2-1-10(26)28-5-7-12(21)14

**InchiKey:** BDDSAMTTYHSXNH-OWOJBTEDSA-N

**Formula:** C17H6Cl3F5O4

**SMILES:** O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 475.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1157.42 | kJ/mol | Joback Method |
| hf | -1413.06 | kJ/mol | Joback Method |
| hfus | 58.52 | kJ/mol | Joback Method |
| hvap | 90.62 | kJ/mol | Joback Method |
| log10ws | -7.58 | | Crippen Method |
| logp | 5.547 | | Crippen Method |
| mcvol | 259.020 | ml/mol | McGowan Method |
| pc | 1600.00 | kPa | Joback Method |
| rinpol | 2536.00 | | NIST Webbook |
| rinpol | 2536.00 | | NIST Webbook |
| tb | 946.94 | K | Joback Method |
| tc | 1168.90 | K | Joback Method |
| tf | 666.30 | K | Joback Method |
| vc | 1.036 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 669.87 | J/mol×K | 946.94 | Joback Method |
| cpg | 676.87 | J/mol×K | 983.93 | Joback Method |
| cpg | 682.93 | J/mol×K | 1020.93 | Joback Method |
| cpg | 688.06 | J/mol×K | 1057.92 | Joback Method |
| cpg | 692.26 | J/mol×K | 1094.91 | Joback Method |
| cpg | 695.54 | J/mol×K | 1131.90 | Joback Method |
| cpg | 697.91 | J/mol×K | 1168.90 | Joback Method |

# Sources

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|---|---|
| **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=U405886&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |