# Succinic acid, 3-chlorophenyl pentafluorobenzyl ester

**Inchi:** InChI=1S/C17H10ClF5O4/c18-8-2-1-3-9(6-8)27-12(25)5-4-11(24)26-7-10-13(19)15(21)1

**InchiKey:** WYUMACPUACBMAF-UHFFFAOYSA-N

**Formula:** C17H10ClF5O4

**SMILES:** O=C(CCC(=O)Oc1cccc(Cl)c1)OCc1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 408.70

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1194.52 | kJ/mol | Joback Method |
| hf | -1475.86 | kJ/mol | Joback Method |
| hfus | 50.70 | kJ/mol | Joback Method |
| hvap | 80.57 | kJ/mol | Joback Method |
| log10ws | -6.36 | | Crippen Method |
| logp | 4.465 | | Crippen Method |
| mcvol | 238.840 | ml/mol | McGowan Method |
| pc | 1668.70 | kPa | Joback Method |
| rinpol | 2315.00 | | NIST Webbook |
| rinpol | 2315.00 | | NIST Webbook |
| tb | 857.96 | K | Joback Method |
| tc | 1064.21 | K | Joback Method |
| tf | 586.50 | K | Joback Method |
| vc | 0.959 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 665.41 | J/mol×K | 857.96 | Joback Method |
| cpg | 675.19 | J/mol×K | 892.33 | Joback Method |
| cpg | 684.03 | J/mol×K | 926.71 | Joback Method |
| cpg | 691.93 | J/mol×K | 961.08 | Joback Method |
| cpg | 698.89 | J/mol×K | 995.46 | Joback Method |
| cpg | 704.91 | J/mol×K | 1029.83 | Joback Method |
| cpg | 709.99 | J/mol×K | 1064.21 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U389888&Units=SI |

# 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 |