# Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-isopropoxyphenyl ester

**Inchi:** InChI=1S/C18H18F8O5/c1-10(2)30-11-5-3-4-6-12(11)31-14(28)8-7-13(27)29-9-16(21,22
**InchiKey:** TXDRSTGFOJNVIM-UHFFFAOYSA-N
**Formula:** C18H18F8O5
**SMILES:** CC(C)Oc1ccccc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
**Mol. weight [g/mol]:** 466.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1924.22 | kJ/mol | Joback Method |
| hf | -2417.30 | kJ/mol | Joback Method |
| hfus | 38.14 | kJ/mol | Joback Method |
| hvap | 68.12 | kJ/mol | Joback Method |
| log10ws | -5.90 | | Crippen Method |
| logp | 4.874 | | Crippen Method |
| mcvol | 275.630 | ml/mol | McGowan Method |
| pc | 1238.09 | kPa | Joback Method |
| rinpol | 1980.00 | | NIST Webbook |
| rinpol | 1980.00 | | NIST Webbook |
| tb | 801.49 | K | Joback Method |
| tc | 986.85 | K | Joback Method |
| tf | 480.09 | K | Joback Method |
| vc | 1.101 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 855.77 | J/mol×K | 801.49 | Joback Method |
| cpg | 868.47 | J/mol×K | 832.38 | Joback Method |
| cpg | 880.22 | J/mol×K | 863.28 | Joback Method |
| cpg | 891.05 | J/mol×K | 894.17 | Joback Method |
| cpg | 901.03 | J/mol×K | 925.06 | Joback Method |
| cpg | 910.21 | J/mol×K | 955.96 | Joback Method |
| cpg | 918.62 | J/mol×K | 986.85 | 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=U389785&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 |