# Succinic acid, pentyl 2-(trifluoromethyl)benzyl ester

**Inchi:** InChI=1S/C17H21F3O4/c1-2-3-6-11-23-15(21)9-10-16(22)24-12-13-7-4-5-8-14(13)17(18

**InchiKey:** SMVADXTWJCBFSA-UHFFFAOYSA-N

**Formula:** C17H21F3O4

**SMILES:** CCCCCOC(=O)CCC(=O)OCc1ccccc1C(F)(F)F

**Mol. weight [g/mol]:** 346.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -854.39 | kJ/mol | Joback Method |
| hf | -1255.83 | kJ/mol | Joback Method |
| hfus | 40.84 | kJ/mol | Joback Method |
| hvap | 70.94 | kJ/mol | Joback Method |
| log10ws | -4.95 | | Crippen Method |
| logp | 4.262 | | Crippen Method |
| mcvol | 246.820 | ml/mol | McGowan Method |
| pc | 1528.27 | kPa | Joback Method |
| rinpol | 2020.00 | | NIST Webbook |
| rinpol | 2020.00 | | NIST Webbook |
| tb | 767.18 | K | Joback Method |
| tc | 957.59 | K | Joback Method |
| tf | 468.80 | K | Joback Method |
| vc | 0.971 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 729.19 | J/mol×K | 767.18 | Joback Method |
| cpg | 743.32 | J/mol×K | 798.92 | Joback Method |
| cpg | 756.53 | J/mol×K | 830.65 | Joback Method |
| cpg | 768.84 | J/mol×K | 862.39 | Joback Method |
| cpg | 780.28 | J/mol×K | 894.12 | Joback Method |
| cpg | 790.87 | J/mol×K | 925.86 | Joback Method |
| cpg | 800.66 | J/mol×K | 957.59 | Joback Method |

# Sources

| | |
|---|---|
| **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=U381653&Units=SI |

# Legend

| | |
|---|---|
| **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 |

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