# Succinic acid, decyl 2,3,6-trifluorobenzyl ester

**Inchi:** InChI=1S/C21H29F3O4/c1-2-3-4-5-6-7-8-9-14-27-19(25)12-13-20(26)28-15-16-17(22)10
**InchiKey:** XUDWSMJWYFWBBB-UHFFFAOYSA-N
**Formula:** C21H29F3O4
**SMILES:** CCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)ccc(F)c1F
**Mol. weight [g/mol]:** 402.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -842.81 | kJ/mol | Joback Method |
| hf | -1352.58 | kJ/mol | Joback Method |
| hfus | 57.83 | kJ/mol | Joback Method |
| hvap | 82.46 | kJ/mol | Joback Method |
| log10ws | -6.93 | | Crippen Method |
| logp | 5.611 | | Crippen Method |
| mcvol | 303.180 | ml/mol | McGowan Method |
| pc | 1117.81 | kPa | Joback Method |
| rinpol | 2515.00 | | NIST Webbook |
| rinpol | 2515.00 | | NIST Webbook |
| tb | 871.89 | K | Joback Method |
| tc | 1068.26 | K | Joback Method |
| tf | 536.50 | K | Joback Method |
| vc | 1.206 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 957.66 | J/mol×K | 871.89 | Joback Method |
| cpg | 973.00 | J/mol×K | 904.62 | Joback Method |
| cpg | 987.21 | J/mol×K | 937.35 | Joback Method |
| cpg | 1000.32 | J/mol×K | 970.08 | Joback Method |
| cpg | 1012.33 | J/mol×K | 1002.80 | Joback Method |
| cpg | 1023.27 | J/mol×K | 1035.53 | Joback Method |
| cpg | 1033.14 | J/mol×K | 1068.26 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381181&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 |

# 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 |