# Succinic acid, 1,1,1-trifluoroprop-2-yl heptadecyl ester

**Inchi:** InChI=1S/C24H43F3O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-30-22(28)18-19-2

**InchiKey:** HRFQQHIRFGGXGP-UHFFFAOYSA-N

**Formula:** C24H43F3O4

**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OC(C)C(F)(F)F

**Mol. weight [g/mol]:** 452.59

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -900.67 | kJ/mol | Joback Method |
| hf | -1630.65 | kJ/mol | Joback Method |
| hfus | 61.79 | kJ/mol | Joback Method |
| hvap | 83.19 | kJ/mol | Joback Method |
| log10ws | -8.37 | | Crippen Method |
| logp | 7.675 | | Crippen Method |
| mcvol | 369.210 | ml/mol | McGowan Method |
| pc | 798.89 | kPa | Joback Method |
| rinpol | 2562.00 | | NIST Webbook |
| rinpol | 2562.00 | | NIST Webbook |
| tb | 895.24 | K | Joback Method |
| tc | 1099.65 | K | Joback Method |
| tf | 493.75 | K | Joback Method |
| vc | 1.464 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1239.26 | J/mol×K | 895.24 | Joback Method |
| cpg | 1259.04 | J/mol×K | 929.31 | Joback Method |
| cpg | 1277.45 | J/mol×K | 963.38 | Joback Method |
| cpg | 1294.54 | J/mol×K | 997.45 | Joback Method |
| cpg | 1310.37 | J/mol×K | 1031.51 | Joback Method |
| cpg | 1324.99 | J/mol×K | 1065.58 | Joback Method |
| cpg | 1338.46 | J/mol×K | 1099.65 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390887&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 |