# Succinic acid, 1,1,1-trifluoroprop-2-yl hex-5-en-1-yl ester

**Inchi:** InChI=1S/C13H19F3O4/c1-3-4-5-6-9-19-11(17)7-8-12(18)20-10(2)13(14,15)16/h3,10H,1

**InchiKey:** VJCBFUVHUNZZTE-UHFFFAOYSA-N

**Formula:** C13H19F3O4

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

**Mol. weight [g/mol]:** 296.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -905.45 | kJ/mol | Joback Method |
| hf | -1278.18 | kJ/mol | Joback Method |
| hfus | 32.02 | kJ/mol | Joback Method |
| hvap | 58.04 | kJ/mol | Joback Method |
| log10ws | -3.62 | | Crippen Method |
| logp | 3.160 | | Crippen Method |
| mcvol | 209.920 | ml/mol | McGowan Method |
| pc | 1679.66 | kPa | Joback Method |
| rinpol | 1485.00 | | NIST Webbook |
| rinpol | 1485.00 | | NIST Webbook |
| tb | 640.24 | K | Joback Method |
| tc | 810.79 | K | Joback Method |
| tf | 368.02 | K | Joback Method |
| vc | 0.830 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 573.23 | J/mol×K | 640.24 | Joback Method |
| cpg | 586.91 | J/mol×K | 668.67 | Joback Method |
| cpg | 599.90 | J/mol×K | 697.09 | Joback Method |
| cpg | 612.21 | J/mol×K | 725.52 | Joback Method |
| cpg | 623.86 | J/mol×K | 753.94 | Joback Method |
| cpg | 634.88 | J/mol×K | 782.37 | Joback Method |
| cpg | 645.27 | J/mol×K | 810.79 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391275&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |