# Succinic acid, 1,1,1-trifluoroprop-2-yl 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C16H23F3O4/c1-5-6-7-13(10-11(2)3)23-15(21)9-8-14(20)22-12(4)16(17,18)19

**InchiKey:** XVUHNTLXOSBZKB-UHFFFAOYSA-N

**Formula:** C16H23F3O4

**SMILES:** CCC#CC(CC(C)C)OC(=O)CCC(=O)OC(C)C(F)(F)F

**Mol. weight [g/mol]:** 336.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -770.11 | kJ/mol | Joback Method |
| hf | -1203.79 | kJ/mol | Joback Method |
| hfus | 37.15 | kJ/mol | Joback Method |
| hvap | 66.76 | kJ/mol | Joback Method |
| log10ws | -4.68 | | Crippen Method |
| logp | 3.632 | | Crippen Method |
| mcvol | 247.890 | ml/mol | McGowan Method |
| pc | 1486.14 | kPa | Joback Method |
| rinpol | 1637.00 | | NIST Webbook |
| rinpol | 1637.00 | | NIST Webbook |
| tb | 720.32 | K | Joback Method |
| tc | 906.07 | K | Joback Method |
| tf | 479.69 | K | Joback Method |
| vc | 0.967 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 715.10 | J/mol×K | 720.32 | Joback Method |
| cpg | 730.39 | J/mol×K | 751.28 | Joback Method |
| cpg | 744.80 | J/mol×K | 782.24 | Joback Method |
| cpg | 758.35 | J/mol×K | 813.20 | Joback Method |
| cpg | 771.05 | J/mol×K | 844.16 | Joback Method |
| cpg | 782.94 | J/mol×K | 875.11 | Joback Method |
| cpg | 794.03 | J/mol×K | 906.07 | Joback Method |

# Sources

| | |
|---|---|
| **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=U391022&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 |