

Succinic acid, 2,2,3,3-tetrafluoropropyl 2-methyloct-5-yn-4-yl ester

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|----------------------|-----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C16H22F4O4/c1-4-5-6-12(9-11(2)3)24-14(22)8-7-13(21)23-10-16(19,20)15(17) |
| InchiKey: | CGIPKBVFAPODDJ-UHFFFAOYSA-N |
| Formula: | C16H22F4O4 |
| SMILES: | CCC#CC(CC(C)C)OC(=O)CCC(=O)OCC(F)(F)C(F)F |
| Mol. weight [g/mol]: | 354.34 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -964.92 | kJ/mol | Joback Method |
| hf | -1399.90 | kJ/mol | Joback Method |
| hfus | 40.23 | kJ/mol | Joback Method |
| hvap | 65.95 | kJ/mol | Joback Method |
| log10ws | -4.54 | | Crippen Method |
| logp | 3.582 | | Crippen Method |
| mvol | 249.660 | ml/mol | McGowan Method |
| pc | 1435.89 | kPa | Joback Method |
| rinpol | 1707.00 | | NIST Webbook |
| rinpol | 1707.00 | | NIST Webbook |
| tb | 719.59 | K | Joback Method |
| tc | 900.12 | K | Joback Method |
| tf | 480.28 | K | Joback Method |
| vc | 0.985 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 722.89 | J/mol×K | 719.59 | Joback Method |
| cpg | 737.69 | J/mol×K | 749.68 | Joback Method |
| cpg | 751.64 | J/mol×K | 779.77 | Joback Method |
| cpg | 764.78 | J/mol×K | 809.86 | Joback Method |
| cpg | 777.11 | J/mol×K | 839.95 | Joback Method |
| cpg | 788.66 | J/mol×K | 870.03 | Joback Method |
| cpg | 799.45 | J/mol×K | 900.12 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391023&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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

| | |
|-----------------|-------------------------------------------------|
| 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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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