

Succinic acid, 2,2,3,3-tetrafluoropropyl 2-hexyl ester

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| Inchi: | InChI=1S/C13H20F4O4/c1-3-4-5-9(2)21-11(19)7-6-10(18)20-8-13(16,17)12(14)15/h9,12 |
| InchiKey: | CGALUNFNQICVGU-UHFFFAOYSA-N |
| Formula: | C13H20F4O4 |
| SMILES: | CCCCC(C)OC(=O)CCC(=O)OCC(F)(F)C(F)F |
| Mol. weight [g/mol]: | 316.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -1190.54 | kJ/mol | Joback Method |
| hf | -1605.00 | kJ/mol | Joback Method |
| hfus | 32.86 | kJ/mol | Joback Method |
| hvap | 57.50 | kJ/mol | Joback Method |
| log10ws | -3.73 | | Crippen Method |
| logp | 3.332 | | Crippen Method |
| mvol | 215.990 | ml/mol | McGowan Method |
| pc | 1575.95 | kPa | Joback Method |
| rinpol | 1472.00 | | NIST Webbook |
| rinpol | 1472.00 | | NIST Webbook |
| tb | 642.39 | K | Joback Method |
| tc | 807.96 | K | Joback Method |
| tf | 355.37 | K | Joback Method |
| vc | 0.861 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 604.03 | J/mol×K | 642.39 | Joback Method |
| cpg | 617.98 | J/mol×K | 669.98 | Joback Method |
| cpg | 631.26 | J/mol×K | 697.58 | Joback Method |
| cpg | 643.86 | J/mol×K | 725.17 | Joback Method |
| cpg | 655.81 | J/mol×K | 752.77 | Joback Method |
| cpg | 667.12 | J/mol×K | 780.36 | Joback Method |
| cpg | 677.80 | J/mol×K | 807.96 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390677&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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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