

Succinic acid, 2-fluorophenyl hex-5-en-1-yl ester

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|----------------------|---|
| Inchi: | InChI=1S/C16H19FO4/c1-2-3-4-7-12-20-15(18)10-11-16(19)21-14-9-6-5-8-13(14)17/h2,5 |
| InchiKey: | XDQGNFVRLPKDZ-UHFFFAOYSA-N |
| Formula: | C16H19FO4 |
| SMILES: | C=CCCCCOC(=O)CCC(=O)Oc1ccccc1F |
| Mol. weight [g/mol]: | 294.32 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -388.19 | kJ/mol | Joback Method |
| hf | -708.79 | kJ/mol | Joback Method |
| hfus | 38.22 | kJ/mol | Joback Method |
| hvap | 70.97 | kJ/mol | Joback Method |
| log10ws | -4.18 | | Crippen Method |
| logp | 3.411 | | Crippen Method |
| mvol | 224.890 | ml/mol | McGowan Method |
| pc | 1812.32 | kPa | Joback Method |
| rinpol | 2069.00 | | NIST Webbook |
| rinpol | 2069.00 | | NIST Webbook |
| tb | 745.67 | K | Joback Method |
| tc | 943.52 | K | Joback Method |
| tf | 452.17 | K | Joback Method |
| vc | 0.871 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 631.21 | J/molxK | 745.67 | Joback Method |
| cpg | 645.23 | J/molxK | 778.65 | Joback Method |
| cpg | 658.36 | J/molxK | 811.62 | Joback Method |
| cpg | 670.60 | J/molxK | 844.60 | Joback Method |
| cpg | 681.96 | J/molxK | 877.57 | Joback Method |
| cpg | 692.47 | J/molxK | 910.55 | Joback Method |
| cpg | 702.15 | J/molxK | 943.52 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391283&Units=SI |

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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