

# Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-pentyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C14H18F8O4/c1-3-4-8(2)26-10(24)6-5-9(23)25-7-12(17,18)14(21,22)13(19,20) |
| <b>InchiKey:</b>            | NGHKANPFEYCOCN-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C14H18F8O4  |
| <b>SMILES:</b>              | CCCC(C)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)                         |
| <b>Mol. weight [g/mol]:</b> | 402.28  |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -1955.68 | kJ/mol               | Joback Method  |
| hf            | -2427.58 | kJ/mol               | Joback Method  |
| hfus          | 32.94    | kJ/mol               | Joback Method  |
| hvap          | 53.87    | kJ/mol               | Joback Method  |
| log10ws       | -4.78    |                      | Crippen Method |
| logp          | 4.213    |                      | Crippen Method |
| mcvol         | 237.160  | ml/mol               | McGowan Method |
| pc            | 1315.61  | kPa                  | Joback Method  |
| rinpol        | 1475.00  |                      | NIST Webbook   |
| rinpol        | 1475.00  |                      | NIST Webbook   |
| tb            | 655.89   | K                    | Joback Method  |
| tc            | 814.74   | K                    | Joback Method  |
| tf            | 373.84   | K                    | Joback Method  |
| vc            | 0.967    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 694.55 | J/mol×K | 655.89          | Joback Method |
| cpg           | 707.97 | J/mol×K | 682.36          | Joback Method |
| cpg           | 720.63 | J/mol×K | 708.84          | Joback Method |
| cpg           | 732.55 | J/mol×K | 735.31          | Joback Method |
| cpg           | 743.78 | J/mol×K | 761.79          | Joback Method |
| cpg           | 754.34 | J/mol×K | 788.26          | Joback Method |
| cpg           | 764.27 | J/mol×K | 814.74          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U370894&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370894&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

# Legend

|                  |   |
|------------------|---|
| <b>cpg:</b>      | Ideal gas heat capacity                         |
| <b>gf:</b>       | Standard Gibbs free energy of formation         |
| <b>hf:</b>       | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>     | Enthalpy of fusion at standard conditions       |
| <b>h vap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b>  | Log10 of Water solubility in mol/l              |
| <b>logp:</b>     | Octanol/Water partition coefficient             |
| <b>mcvol:</b>    | McGowan's characteristic volume                 |
| <b>pc:</b>       | Critical Pressure                               |
| <b>r in pol:</b> | Non-polar retention indices                     |
| <b>tb:</b>       | Normal Boiling Point Temperature                |
| <b>tc:</b>       | Critical Temperature                            |
| <b>tf:</b>       | Normal melting (fusion) point                   |
| <b>vc:</b>       | Critical Volume                                 |

Latest version available from:

<https://www.cheméo.com/cid/119-567-1/Succinic-acid-2-2-3-3-4-4-5-5-octafluoropentyl-2-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-27 16:16:33.259719217 +0000 UTC m=+16523842.180296544.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.