

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

**Inchi:** InChI=1S/C14H18F8O4/c1-3-8(4-2)26-10(24)6-5-9(23)25-7-12(17,18)14(21,22)13(19,20)  
**InchiKey:** GKUOYBJCMBSDRN-UHFFFAOYSA-N  
**Formula:** C14H18F8O4  
**SMILES:** CCC(CC)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F  
**Mol. weight [g/mol]:** 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        | 1482.00  |         | NIST Webbook   |
| rinpol        | 1482.00  |         | NIST Webbook   |
| tb            | 655.89   | K       | Joback Method  |
| tc            | 814.74   | K       | Joback Method  |
| tf            | 373.84   | K       | Joback Method  |
| vc            | 0.967    | m3/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>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U370926&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370926&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <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>                     |

# 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>hvap:</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>rlnpol:</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                                 |

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