

# Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3,3-dimethylbut-2-yl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C15H20F8O4/c1-8(12(2,3)4)27-10(25)6-5-9(24)26-7-13(18,19)15(22,23)14(20) |
| <b>InchiKey:</b>            | FNPFWBELIHXNS-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C15H20F8O4  |
| <b>SMILES:</b>              | CC(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)C(C)C)                          |
| <b>Mol. weight [g/mol]:</b> | 416.30  |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -1944.42 | kJ/mol               | Joback Method  |
| hf            | -2456.97 | kJ/mol               | Joback Method  |
| hfus          | 28.12    | kJ/mol               | Joback Method  |
| hvap          | 54.80    | kJ/mol               | Joback Method  |
| log10ws       | -4.95    |                      | Crippen Method |
| logp          | 4.459    |                      | Crippen Method |
| mcvol         | 251.250  | ml/mol               | McGowan Method |
| pc            | 1245.09  | kPa                  | Joback Method  |
| rinpol        | 1510.00  |                      | NIST Webbook   |
| rinpol        | 1510.00  |                      | NIST Webbook   |
| tb            | 675.54   | K                    | Joback Method  |
| tc            | 839.81   | K                    | Joback Method  |
| tf            | 387.53   | K                    | Joback Method  |
| vc            | 1.012    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 751.00 | J/mol×K | 675.54          | Joback Method |
| cpg           | 765.05 | J/mol×K | 702.92          | Joback Method |
| cpg           | 778.24 | J/mol×K | 730.30          | Joback Method |
| cpg           | 790.62 | J/mol×K | 757.67          | Joback Method |
| cpg           | 802.22 | J/mol×K | 785.05          | Joback Method |
| cpg           | 813.10 | J/mol×K | 812.43          | Joback Method |
| cpg           | 823.30 | J/mol×K | 839.81          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U390616&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390616&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>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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                                 |

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