

# Sebacic acid, pentafluorobenzyl tridecyl ester

**Inchi:** InChI=1S/C30H45F5O4/c1-2-3-4-5-6-7-8-9-12-15-18-21-38-24(36)19-16-13-10-11-14-17  
**InchiKey:** FYIMYCCUNFPASJ-UHFFFAOYSA-N  
**Formula:** C30H45F5O4  
**SMILES:** CCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 564.67

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -1175.91 | kJ/mol  | Joback Method  |
| hf            | -1953.50 | kJ/mol  | Joback Method  |
| hfus          | 86.53    | kJ/mol  | Joback Method  |
| hvap          | 102.19   | kJ/mol  | Joback Method  |
| log10ws       | -11.36   |         | Crippen Method |
| logp          | 9.400    |         | Crippen Method |
| mcvol         | 433.530  | ml/mol  | McGowan Method |
| pc            | 632.89   | kPa     | Joback Method  |
| rinpol        | 3380.00  |         | NIST Webbook   |
| tb            | 1086.31  | K       | Joback Method  |
| tc            | 1384.50  | K       | Joback Method  |
| tf            | 664.15   | K       | Joback Method  |
| vc            | 1.746    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1525.47 | J/mol×K | 1086.31         | Joback Method |
| cpg           | 1545.10 | J/mol×K | 1136.01         | Joback Method |
| cpg           | 1561.64 | J/mol×K | 1185.71         | Joback Method |
| cpg           | 1575.19 | J/mol×K | 1235.41         | Joback Method |
| cpg           | 1585.88 | J/mol×K | 1285.10         | Joback Method |
| cpg           | 1593.80 | J/mol×K | 1334.80         | Joback Method |
| cpg           | 1599.06 | J/mol×K | 1384.50         | 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=U354908&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354908&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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>rinpol:</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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