# Sebacic acid, undecyl 1-phenyl-2,2,2-trifluoromethylethyl ester

**Inchi:** InChI=1S/C29H45F3O4/c1-2-3-4-5-6-7-10-13-19-24-35-26(33)22-17-11-8-9-12-18-23-27

**InchiKey:** YJLBGUSDJCRPFW-UHFFFAOYSA-N

**Formula:** C29H45F3O4

**SMILES:** CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(c1ccccc1)C(F)(F)F

**Mol. weight [g/mol]:** 514.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -746.16 | kJ/mol | Joback Method |
| hf | -1497.32 | kJ/mol | Joback Method |
| hfus | 68.78 | kJ/mol | Joback Method |
| hvap | 96.60 | kJ/mol | Joback Method |
| log10ws | -9.91 | | Crippen Method |
| logp | 9.028 | | Crippen Method |
| mcvol | 415.900 | ml/mol | McGowan Method |
| pc | 735.62 | kPa | Joback Method |
| rinpol | 2964.00 | | NIST Webbook |
| rinpol | 2964.00 | | NIST Webbook |
| tb | 1036.32 | K | Joback Method |
| tc | 1282.35 | K | Joback Method |
| tf | 576.52 | K | Joback Method |
| vc | 1.637 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1453.49 | J/mol×K | 1036.32 | Joback Method |
| cpg | 1472.40 | J/mol×K | 1077.33 | Joback Method |
| cpg | 1489.56 | J/mol×K | 1118.33 | Joback Method |
| cpg | 1505.13 | J/mol×K | 1159.34 | Joback Method |
| cpg | 1519.22 | J/mol×K | 1200.34 | Joback Method |
| cpg | 1531.98 | J/mol×K | 1241.35 | Joback Method |
| cpg | 1543.53 | J/mol×K | 1282.35 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=U416808&Units=SI |

# Legend

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|---|---|
| **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 |
| **hvap:** | 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |