# Sebacic acid, pentafluorobenzyl tetradecyl ester

**Inchi:** InChI=1S/C31H47F5O4/c1-2-3-4-5-6-7-8-9-10-13-16-19-22-39-25(37)20-17-14-11-12-15

**InchiKey:** LLZLRACQBUCWMU-UHFFFAOYSA-N

**Formula:** C31H47F5O4

**SMILES:** CCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 578.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1167.49 | kJ/mol | Joback Method |
| hf | -1974.14 | kJ/mol | Joback Method |
| hfus | 89.12 | kJ/mol | Joback Method |
| hvap | 104.41 | kJ/mol | Joback Method |
| log10ws | -11.78 | | Crippen Method |
| logp | 9.790 | | Crippen Method |
| mcvol | 447.620 | ml/mol | McGowan Method |
| pc | 603.39 | kPa | Joback Method |
| rinpol | 3483.00 | | NIST Webbook |
| rinpol | 3483.00 | | NIST Webbook |
| tb | 1109.19 | K | Joback Method |
| tc | 1426.64 | K | Joback Method |
| tf | 675.42 | K | Joback Method |
| vc | 1.802 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1588.67 | J/mol×K | 1109.19 | Joback Method |
| cpg | 1608.86 | J/mol×K | 1162.10 | Joback Method |
| cpg | 1625.54 | J/mol×K | 1215.01 | Joback Method |
| cpg | 1638.85 | J/mol×K | 1267.92 | Joback Method |
| cpg | 1648.93 | J/mol×K | 1320.82 | Joback Method |
| cpg | 1655.93 | J/mol×K | 1373.73 | Joback Method |
| cpg | 1659.98 | J/mol×K | 1426.64 | Joback Method |

# Sources

| | |
|---|---|
| **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=U354909&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |