# Pimelic acid, pentafluorobenzyl tetradecyl ester

**Inchi:** InChI=1S/C28H41F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-36-22(34)17-14-13-15-18-23

**InchiKey:** KYGXLCJSSBDFOJ-UHFFFAOYSA-N

**Formula:** C28H41F5O4

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

**Mol. weight [g/mol]:** 536.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1192.75 | kJ/mol | Joback Method |
| hf | -1912.22 | kJ/mol | Joback Method |
| hfus | 81.35 | kJ/mol | Joback Method |
| hvap | 97.73 | kJ/mol | Joback Method |
| log10ws | -10.52 | | Crippen Method |
| logp | 8.620 | | Crippen Method |
| mcvol | 405.350 | ml/mol | McGowan Method |
| pc | 698.76 | kPa | Joback Method |
| rinpol | 3192.00 | | NIST Webbook |
| rinpol | 3192.00 | | NIST Webbook |
| tb | 1040.55 | K | Joback Method |
| tc | 1305.98 | K | Joback Method |
| tf | 641.61 | K | Joback Method |
| vc | 1.633 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1399.67 | J/mol×K | 1040.55 | Joback Method |
| cpg | 1418.18 | J/mol×K | 1084.79 | Joback Method |
| cpg | 1434.27 | J/mol×K | 1129.03 | Joback Method |
| cpg | 1448.01 | J/mol×K | 1173.27 | Joback Method |
| cpg | 1459.46 | J/mol×K | 1217.51 | Joback Method |
| cpg | 1468.70 | J/mol×K | 1261.74 | Joback Method |
| cpg | 1475.77 | J/mol×K | 1305.98 | Joback Method |

# Sources

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|---|---|
| **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=U416638&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |