# Phthalic acid, 2,2,3,3,4,4,4-heptafluorobutyl tridecyl ester

**Inchi:** InChI=1S/C25H33F7O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-35-21(33)19-15-12-13-16-20(19

**InchiKey:** GWQTTZHHABXYIZ-UHFFFAOYSA-N

**Formula:** C25H33F7O4

**SMILES:** CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 530.52

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1560.59 | kJ/mol | Joback Method |
| hf | -2222.89 | kJ/mol | Joback Method |
| hfus | 59.05 | kJ/mol | Joback Method |
| hvap | 82.89 | kJ/mol | Joback Method |
| log10ws | -9.53 | | Crippen Method |
| logp | 8.144 | | Crippen Method |
| mcvol | 366.620 | ml/mol | McGowan Method |
| pc | 831.46 | kPa | Joback Method |
| rinpol | 2607.00 | | NIST Webbook |
| tb | 940.84 | K | Joback Method |
| tc | 1154.86 | K | Joback Method |
| tf | 566.16 | K | Joback Method |
| vc | 1.468 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1230.15 | J/mol×K | 940.84 | Joback Method |
| cpg | 1246.41 | J/mol×K | 976.51 | Joback Method |
| cpg | 1261.50 | J/mol×K | 1012.18 | Joback Method |
| cpg | 1275.54 | J/mol×K | 1047.85 | Joback Method |
| cpg | 1288.64 | J/mol×K | 1083.52 | Joback Method |
| cpg | 1300.91 | J/mol×K | 1119.19 | Joback Method |
| cpg | 1312.47 | J/mol×K | 1154.86 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415551&Units=SI |
| **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 |

# 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 |