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

**Inchi:** InChI=1S/C22H27F7O4/c1-2-3-4-5-6-7-8-11-14-32-18(30)16-12-9-10-13-17(16)19(31)33

**InchiKey:** YVIITHYTNXIEQY-UHFFFAOYSA-N

**Formula:** C22H27F7O4

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

**Mol. weight [g/mol]:** 488.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1585.85 | kJ/mol | Joback Method |
| hf | -2160.97 | kJ/mol | Joback Method |
| hfus | 51.28 | kJ/mol | Joback Method |
| hvap | 76.21 | kJ/mol | Joback Method |
| log10ws | -8.27 | | Crippen Method |
| logp | 6.974 | | Crippen Method |
| mcvol | 324.350 | ml/mol | McGowan Method |
| pc | 988.88 | kPa | Joback Method |
| rinpol | 2317.00 | | NIST Webbook |
| rinpol | 2317.00 | | NIST Webbook |
| tb | 872.20 | K | Joback Method |
| tc | 1067.96 | K | Joback Method |
| tf | 532.35 | K | Joback Method |
| vc | 1.300 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1049.79 | J/mol×K | 872.20 | Joback Method |
| cpg | 1064.46 | J/mol×K | 904.83 | Joback Method |
| cpg | 1078.11 | J/mol×K | 937.45 | Joback Method |
| cpg | 1090.81 | J/mol×K | 970.08 | Joback Method |
| cpg | 1102.65 | J/mol×K | 1002.71 | Joback Method |
| cpg | 1113.70 | J/mol×K | 1035.34 | Joback Method |
| cpg | 1124.05 | J/mol×K | 1067.96 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415548&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |