# Terephthalic acid, heptyl 2,2,3,3,3-pentafluoropropyl ester

**Inchi:** InChI=1S/C18H21F5O4/c1-2-3-4-5-6-11-26-15(24)13-7-9-14(10-8-13)16(25)27-12-17(19

**InchiKey:** SHHLMRNRBRZARP-UHFFFAOYSA-N

**Formula:** C18H21F5O4

**SMILES:** CCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)(F)F)cc1

**Mol. weight [g/mol]:** 396.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1232.75 | kJ/mol | Joback Method |
| hf | -1677.44 | kJ/mol | Joback Method |
| hfus | 42.17 | kJ/mol | Joback Method |
| hvap | 70.23 | kJ/mol | Joback Method |
| log10ws | -6.28 | | Crippen Method |
| logp | 5.168 | | Crippen Method |
| mcvol | 264.450 | ml/mol | McGowan Method |
| pc | 1346.69 | kPa | Joback Method |
| rinpol | 2088.00 | | NIST Webbook |
| rinpol | 2088.00 | | NIST Webbook |
| tb | 785.37 | K | Joback Method |
| tc | 972.53 | K | Joback Method |
| tf | 483.67 | K | Joback Method |
| vc | 1.052 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 802.42 | J/mol×K | 785.37 | Joback Method |
| cpg | 816.18 | J/mol×K | 816.56 | Joback Method |
| cpg | 829.01 | J/mol×K | 847.76 | Joback Method |
| cpg | 840.95 | J/mol×K | 878.95 | Joback Method |
| cpg | 852.05 | J/mol×K | 910.14 | Joback Method |
| cpg | 862.35 | J/mol×K | 941.34 | Joback Method |
| cpg | 871.90 | J/mol×K | 972.53 | Joback Method |

# Sources

| | |
|---|---|
| **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=U415778&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 |