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

**Inchi:** InChI=1S/C20H25F5O4/c1-2-3-4-5-6-7-8-13-28-17(26)15-9-11-16(12-10-15)18(27)29-14

**InchiKey:** VOMZPKYFHCASNM-UHFFFAOYSA-N

**Formula:** C20H25F5O4

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

**Mol. weight [g/mol]:** 424.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1215.91 | kJ/mol | Joback Method |
| hf | -1718.72 | kJ/mol | Joback Method |
| hfus | 47.35 | kJ/mol | Joback Method |
| hvap | 74.69 | kJ/mol | Joback Method |
| log10ws | -7.12 | | Crippen Method |
| logp | 5.948 | | Crippen Method |
| mcvol | 292.630 | ml/mol | McGowan Method |
| pc | 1175.24 | kPa | Joback Method |
| rinpol | 2278.00 | | NIST Webbook |
| rinpol | 2278.00 | | NIST Webbook |
| tb | 831.13 | K | Joback Method |
| tc | 1021.80 | K | Joback Method |
| tf | 506.21 | K | Joback Method |
| vc | 1.163 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 916.89 | J/mol×K | 831.13 | Joback Method |
| cpg | 931.33 | J/mol×K | 862.91 | Joback Method |
| cpg | 944.78 | J/mol×K | 894.69 | Joback Method |
| cpg | 957.28 | J/mol×K | 926.47 | Joback Method |
| cpg | 968.90 | J/mol×K | 958.25 | Joback Method |
| cpg | 979.69 | J/mol×K | 990.02 | Joback Method |
| cpg | 989.69 | J/mol×K | 1021.80 | 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=U415780&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 |