# Pentafluorobenzoic acid, 2-pentyl ester

**Other names:** 1-Methylbutyl pentafluorobenzoate
Pentan-2-yl 2,3,4,5,6-pentafluorobenzoate
**Inchi:** InChI=1S/C12H11F5O2/c1-3-4-5(2)19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h5H,3-4H2
**InchiKey:** BKCNCJFSIBDJLT-UHFFFAOYSA-N
**Formula:** C12H11F5O2
**SMILES:** CCCC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 282.21
**CAS:** 99483-15-5

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1095.99 | kJ/mol | Joback Method |
| hf | -1342.46 | kJ/mol | Joback Method |
| hfus | 33.60 | kJ/mol | Joback Method |
| hvap | 52.58 | kJ/mol | Joback Method |
| log10ws | -5.16 | | Crippen Method |
| logp | 3.728 | | Crippen Method |
| mcvol | 172.470 | ml/mol | McGowan Method |
| pc | 1915.26 | kPa | Joback Method |
| rinpol | 1247.00 | | NIST Webbook |
| rinpol | 1277.00 | | NIST Webbook |
| rinpol | 1255.00 | | NIST Webbook |
| rinpol | 1277.00 | | NIST Webbook |
| rinpol | 1253.00 | | NIST Webbook |
| rinpol | 1257.00 | | NIST Webbook |
| rinpol | 1253.00 | | NIST Webbook |
| ripol | 1506.00 | | NIST Webbook |
| ripol | 1518.00 | | NIST Webbook |
| ripol | 1518.00 | | NIST Webbook |
| ripol | 1483.00 | | NIST Webbook |
| ripol | 1506.00 | | NIST Webbook |
| ripol | 1498.00 | | NIST Webbook |
| tb | 597.74 | K | Joback Method |
| tc | 771.09 | K | Joback Method |
| tf | 374.13 | K | Joback Method |
| vc | 0.708 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 433.19 | J/mol×K | 597.74 | Joback Method |
| cpg | 444.56 | J/mol×K | 626.63 | Joback Method |
| cpg | 455.45 | J/mol×K | 655.52 | Joback Method |
| cpg | 465.86 | J/mol×K | 684.41 | Joback Method |
| cpg | 475.78 | J/mol×K | 713.31 | Joback Method |
| cpg | 485.23 | J/mol×K | 742.20 | Joback Method |
| cpg | 494.19 | J/mol×K | 771.09 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C99483155&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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume