# 2-(2-Methoxyethoxy)ethyl 2,3,4,5,6-pentafluorobenzoate

**Inchi:** InChI=1S/C12H11F5O4/c1-19-2-3-20-4-5-21-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h2-5

**InchiKey:** JXOQNHMYTDLJAU-UHFFFAOYSA-N

**Formula:** C12H11F5O4

**SMILES:** COCCOCCOC(=O)c1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 314.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1303.55 | kJ/mol | Joback Method |
| hf | -1601.62 | kJ/mol | Joback Method |
| hfus | 39.49 | kJ/mol | Joback Method |
| hvap | 57.78 | kJ/mol | Joback Method |
| log10ws | -3.22 | | Crippen Method |
| logp | 2.202 | | Crippen Method |
| mcvol | 184.210 | ml/mol | McGowan Method |
| pc | 1846.75 | kPa | Joback Method |
| rinpol | 1537.00 | | NIST Webbook |
| rinpol | 1537.00 | | NIST Webbook |
| tb | 643.02 | K | Joback Method |
| tc | 813.74 | K | Joback Method |
| tf | 433.59 | K | Joback Method |
| vc | 0.750 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 482.50 | J/mol×K | 643.02 | Joback Method |
| cpg | 493.59 | J/mol×K | 671.47 | Joback Method |
| cpg | 504.23 | J/mol×K | 699.93 | Joback Method |
| cpg | 514.39 | J/mol×K | 728.38 | Joback Method |
| cpg | 524.07 | J/mol×K | 756.83 | Joback Method |
| cpg | 533.24 | J/mol×K | 785.29 | Joback Method |
| cpg | 541.88 | J/mol×K | 813.74 | 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=U378301&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

| | |
|---|---|
| **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 |

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