# Isophthalic acid, di(pentafluorobenzyl) ester

**Inchi:** InChI=1S/C22H8F10O4/c23-11-9(12(24)16(28)19(31)15(11)27)5-35-21(33)7-2-1-3-8(4-7
**InchiKey:** KCNITRSOMNWVTA-UHFFFAOYSA-N
**Formula:** C22H8F10O4
**SMILES:** O=C(OCc1c(F)c(F)c(F)c(F)c1F)c1cccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
**Mol. weight [g/mol]:** 526.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2050.28 | kJ/mol | Joback Method |
| hf | -2364.69 | kJ/mol | Joback Method |
| hfus | 66.95 | kJ/mol | Joback Method |
| hvap | 88.82 | kJ/mol | Joback Method |
| log10ws | -9.49 | | Crippen Method |
| logp | 5.792 | | Crippen Method |
| mcvol | 282.140 | ml/mol | McGowan Method |
| pc | 1222.55 | kPa | Joback Method |
| tb | 982.86 | K | Joback Method |
| tc | 1203.41 | K | Joback Method |
| tf | 704.90 | K | Joback Method |
| vc | 1.171 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 847.22 | J/mol×K | 982.86 | Joback Method |
| cpg | 855.09 | J/mol×K | 1019.62 | Joback Method |
| cpg | 861.63 | J/mol×K | 1056.38 | Joback Method |
| cpg | 866.84 | J/mol×K | 1093.14 | Joback Method |
| cpg | 870.72 | J/mol×K | 1129.90 | Joback Method |
| cpg | 873.25 | J/mol×K | 1166.65 | Joback Method |
| cpg | 874.44 | J/mol×K | 1203.41 | 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=U344513&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

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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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |