# Phthalic acid, di(2,5-difluorobenzyl) ester

**Inchi:** InChI=1S/C22H14F4O4/c23-15-5-7-19(25)13(9-15)11-29-21(27)17-3-1-2-4-18(17)22(28)
**InchiKey:** HBMSUTAWAGBVIX-UHFFFAOYSA-N
**Formula:** C22H14F4O4
**SMILES:** O=C(OCc1cc(F)ccc1F)c1ccccc1C(=O)OCc1cc(F)ccc1F
**Mol. weight [g/mol]:** 418.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -823.64 | kJ/mol | Joback Method |
| hf | -1119.21 | kJ/mol | Joback Method |
| hfus | 50.81 | kJ/mol | Joback Method |
| hvap | 89.75 | kJ/mol | Joback Method |
| log10ws | -7.50 | | Crippen Method |
| logp | 4.957 | | Crippen Method |
| mcvol | 271.520 | ml/mol | McGowan Method |
| pc | 1600.00 | kPa | Joback Method |
| rinpol | 2620.00 | | NIST Webbook |
| rinpol | 2620.00 | | NIST Webbook |
| tb | 957.36 | K | Joback Method |
| tc | 1184.98 | K | Joback Method |
| tf | 626.24 | K | Joback Method |
| vc | 1.063 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 815.77 | J/mol×K | 957.36 | Joback Method |
| cpg | 825.73 | J/mol×K | 995.30 | Joback Method |
| cpg | 834.40 | J/mol×K | 1033.23 | Joback Method |
| cpg | 841.81 | J/mol×K | 1071.17 | Joback Method |
| cpg | 848.01 | J/mol×K | 1109.11 | Joback Method |
| cpg | 853.01 | J/mol×K | 1147.04 | Joback Method |
| cpg | 856.85 | J/mol×K | 1184.98 | 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=U377815&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 |