# Isophthalic acid, di(3-fluorophenyl) ester

**Inchi:** InChI=1S/C20H12F2O4/c21-15-6-2-8-17(11-15)25-19(23)13-4-1-5-14(10-13)20(24)26-18
**InchiKey:** KXDSESZJFNCNKF-UHFFFAOYSA-N
**Formula:** C20H12F2O4
**SMILES:** O=C(Oc1cccc(F)c1)c1cccc(C(=O)Oc2cccc(F)c2)c1
**Mol. weight [g/mol]:** 354.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -431.60 | kJ/mol | Joback Method |
| hf | -662.77 | kJ/mol | Joback Method |
| hfus | 40.25 | kJ/mol | Joback Method |
| hvap | 85.61 | kJ/mol | Joback Method |
| log10ws | -6.31 | | Crippen Method |
| logp | 4.403 | | Crippen Method |
| mcvol | 239.800 | ml/mol | McGowan Method |
| pc | 2088.84 | kPa | Joback Method |
| rinpol | 2778.00 | | NIST Webbook |
| rinpol | 2778.00 | | NIST Webbook |
| tb | 903.10 | K | Joback Method |
| tc | 1144.49 | K | Joback Method |
| tf | 577.48 | K | Joback Method |
| vc | 0.915 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 691.87 | J/mol×K | 903.10 | Joback Method |
| cpg | 702.67 | J/mol×K | 943.33 | Joback Method |
| cpg | 712.14 | J/mol×K | 983.56 | Joback Method |
| cpg | 720.31 | J/mol×K | 1023.80 | Joback Method |
| cpg | 727.24 | J/mol×K | 1064.03 | Joback Method |
| cpg | 732.95 | J/mol×K | 1104.26 | Joback Method |
| cpg | 737.51 | J/mol×K | 1144.49 | 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=U344674&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 |