# Isophthalic acid, ethyl 2-nitro-5-fluorophenyl ester

**Inchi:** InChI=1S/C16H12FNO6/c1-2-23-15(19)10-4-3-5-11(8-10)16(20)24-14-9-12(17)6-7-13(14

**InchiKey:** BSNVQFSBVYUNGP-UHFFFAOYSA-N

**Formula:** C16H12FNO6

**SMILES:** CCOC(=O)c1cccc(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])c1

**Mol. weight [g/mol]:** 333.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -347.33 | kJ/mol | Joback Method |
| hf | -631.39 | kJ/mol | Joback Method |
| hfus | 44.13 | kJ/mol | Joback Method |
| hvap | 91.83 | kJ/mol | Joback Method |
| log10ws | -5.20 | | Crippen Method |
| logp | 3.130 | | Crippen Method |
| mcvol | 222.850 | ml/mol | McGowan Method |
| pc | 2315.84 | kPa | Joback Method |
| rinpol | 2540.00 | | NIST Webbook |
| rinpol | 2540.00 | | NIST Webbook |
| tb | 937.47 | K | Joback Method |
| tc | 1183.07 | K | Joback Method |
| tf | 649.00 | K | Joback Method |
| vc | 0.864 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 653.60 | J/mol×K | 937.47 | Joback Method |
| cpg | 662.68 | J/mol×K | 978.40 | Joback Method |
| cpg | 670.47 | J/mol×K | 1019.34 | Joback Method |
| cpg | 676.98 | J/mol×K | 1060.27 | Joback Method |
| cpg | 682.24 | J/mol×K | 1101.20 | Joback Method |
| cpg | 686.27 | J/mol×K | 1142.13 | Joback Method |
| cpg | 689.09 | J/mol×K | 1183.07 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U344415&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

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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 |