# Isophthalic acid, monoamide, N-(2-fluorophenyl)-, nonyl ester

**Inchi:** InChI=1S/C23H28FNO3/c1-2-3-4-5-6-7-10-16-28-23(27)19-13-11-12-18(17-19)22(26)25-

**InchiKey:** ULTQPKRGBQCOTM-UHFFFAOYSA-N

**Formula:** C23H28FNO3

**SMILES:** CCCCCCCCCOC(=O)c1cccc(C(=O)Nc2ccccc2F)c1

**Mol. weight [g/mol]:** 385.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -119.92 | kJ/mol | Joback Method |
| hf | -567.95 | kJ/mol | Joback Method |
| hfus | 55.20 | kJ/mol | Joback Method |
| hvap | 94.19 | kJ/mol | Joback Method |
| log10ws | -7.37 | | Crippen Method |
| logp | 5.985 | | Crippen Method |
| mcvol | 308.170 | ml/mol | McGowan Method |
| pc | 1354.63 | kPa | Joback Method |
| rinpol | 3191.00 | | NIST Webbook |
| rinpol | 3191.00 | | NIST Webbook |
| tb | 968.56 | K | Joback Method |
| tc | 1191.22 | K | Joback Method |
| tf | 602.19 | K | Joback Method |
| vc | 1.190 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 991.61 | J/mol×K | 968.56 | Joback Method |
| cpg | 1005.30 | J/mol×K | 1005.67 | Joback Method |
| cpg | 1017.75 | J/mol×K | 1042.78 | Joback Method |
| cpg | 1029.03 | J/mol×K | 1079.89 | Joback Method |
| cpg | 1039.20 | J/mol×K | 1117.00 | Joback Method |
| cpg | 1048.33 | J/mol×K | 1154.11 | Joback Method |
| cpg | 1056.48 | J/mol×K | 1191.22 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U345783&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 |