# 2,4-Difluorobenzoic acid, 2-nitro-5-fluorophenyl ester

**Inchi:** InChI=1S/C13H6F3NO4/c14-7-1-3-9(10(16)5-7)13(18)21-12-6-8(15)2-4-11(12)17(19)20/h

**InchiKey:** NACJRYOZWYXNCH-UHFFFAOYSA-N

**Formula:** C13H6F3NO4

**SMILES:** O=C(Oc1cc(F)ccc1[N+](=O)[O-])c1ccc(F)cc1F

**Mol. weight [g/mol]:** 297.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -537.92 | kJ/mol | Joback Method |
| hf | -728.36 | kJ/mol | Joback Method |
| hfus | 39.34 | kJ/mol | Joback Method |
| hvap | 75.03 | kJ/mol | Joback Method |
| log10ws | -5.20 | | Crippen Method |
| logp | 3.231 | | Crippen Method |
| mcvol | 176.680 | ml/mol | McGowan Method |
| pc | 2654.29 | kPa | Joback Method |
| rinpol | 1935.00 | | NIST Webbook |
| tb | 796.06 | K | Joback Method |
| tc | 1033.47 | K | Joback Method |
| tf | 556.73 | K | Joback Method |
| vc | 0.708 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 475.61 | J/mol×K | 796.06 | Joback Method |
| cpg | 485.34 | J/mol×K | 835.63 | Joback Method |
| cpg | 494.10 | J/mol×K | 875.20 | Joback Method |
| cpg | 501.94 | J/mol×K | 914.76 | Joback Method |
| cpg | 508.86 | J/mol×K | 954.33 | Joback Method |
| cpg | 514.91 | J/mol×K | 993.90 | Joback Method |
| cpg | 520.09 | J/mol×K | 1033.47 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357601&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |