# 2,5-Di(trifluoromethyl)benzoic acid, 4-nitrophenyl ester

**Inchi:** InChI=1S/C15H7F6NO4/c16-14(17,18)8-1-6-12(15(19,20)21)11(7-8)13(23)26-10-4-2-9(3
**InchiKey:** HQUDURDOGOMJHN-UHFFFAOYSA-N
**Formula:** C15H7F6NO4
**SMILES:** O=C(Oc1ccc([N+](=O)[O-])cc1)c1cc(C(F)(F)F)ccc1C(F)(F)F
**Mol. weight [g/mol]:** 379.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1090.20 | kJ/mol | Joback Method |
| hf | -1364.00 | kJ/mol | Joback Method |
| hfus | 39.32 | kJ/mol | Joback Method |
| hvap | 73.78 | kJ/mol | Joback Method |
| log10ws | -6.42 | | Crippen Method |
| logp | 4.852 | | Crippen Method |
| mcvol | 210.170 | ml/mol | McGowan Method |
| pc | 2038.23 | kPa | Joback Method |
| rinpol | 1966.00 | | NIST Webbook |
| rinpol | 1966.00 | | NIST Webbook |
| tb | 828.19 | K | Joback Method |
| tc | 1053.48 | K | Joback Method |
| tf | 573.36 | K | Joback Method |
| vc | 0.852 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 609.98 | J/mol×K | 828.19 | Joback Method |
| cpg | 619.38 | J/mol×K | 865.74 | Joback Method |
| cpg | 627.87 | J/mol×K | 903.29 | Joback Method |
| cpg | 635.53 | J/mol×K | 940.84 | Joback Method |
| cpg | 642.45 | J/mol×K | 978.38 | Joback Method |
| cpg | 648.72 | J/mol×K | 1015.93 | Joback Method |
| cpg | 654.42 | J/mol×K | 1053.48 | 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=U357749&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 |