# 2,5-Dinitrophenol, isoBOC

**Inchi:** InChI=1S/C11H12N2O7/c1-7(2)6-19-11(14)20-10-5-8(12(15)16)3-4-9(10)13(17)18/h3-5,7
**InchiKey:** SNTPIQZLYCWUPM-UHFFFAOYSA-N
**Formula:** C11H12N2O7
**SMILES:** CC(C)COC(=O)Oc1cc([N+](=O)[O-])ccc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 284.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -135.37 | kJ/mol | Joback Method |
| hf | -460.60 | kJ/mol | Joback Method |
| hfus | 40.68 | kJ/mol | Joback Method |
| hvap | 88.04 | kJ/mol | Joback Method |
| log10ws | -4.17 | | Crippen Method |
| logp | 2.674 | | Crippen Method |
| mcvol | 190.240 | ml/mol | McGowan Method |
| pc | 2735.42 | kPa | Joback Method |
| rinpol | 1984.00 | | NIST Webbook |
| rinpol | 1984.00 | | NIST Webbook |
| tb | 889.67 | K | Joback Method |
| tc | 1140.97 | K | Joback Method |
| tf | 631.80 | K | Joback Method |
| vc | 0.744 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 558.65 | J/mol×K | 889.67 | Joback Method |
| cpg | 568.22 | J/mol×K | 931.55 | Joback Method |
| cpg | 576.57 | J/mol×K | 973.44 | Joback Method |
| cpg | 583.71 | J/mol×K | 1015.32 | Joback Method |
| cpg | 589.66 | J/mol×K | 1057.20 | Joback Method |
| cpg | 594.40 | J/mol×K | 1099.09 | Joback Method |
| cpg | 597.96 | J/mol×K | 1140.97 | Joback Method |

# Sources

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|---|---|
| **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=R234987&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |