# 2,2,2-Trichloroethyl 3,5-dinitrobenzoate

**Other names:** Benzoic acid, 3,5-dinitro, 2,2,2-trichloroethyl ester
**Inchi:** InChI=1S/C9H5Cl3N2O6/c10-9(11,12)4-20-8(15)5-1-6(13(16)17)3-7(2-5)14(18)19/h1-3H
**InchiKey:** BFXMGIIKWMJVFQ-UHFFFAOYSA-N
**Formula:** C9H5Cl3N2O6
**SMILES:** O=C(OCC(Cl)(Cl)Cl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 343.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -77.72 | kJ/mol | Joback Method |
| hf | -337.79 | kJ/mol | Joback Method |
| hfus | 43.01 | kJ/mol | Joback Method |
| hvap | 93.42 | kJ/mol | Joback Method |
| log10ws | -5.00 | | Crippen Method |
| logp | 3.030 | | Crippen Method |
| mcvol | 192.910 | ml/mol | McGowan Method |
| pc | 3076.16 | kPa | Joback Method |
| rinpol | 2136.00 | | NIST Webbook |
| rinpol | 2116.00 | | NIST Webbook |
| rinpol | 2105.00 | | NIST Webbook |
| rinpol | 2149.00 | | NIST Webbook |
| tb | 930.99 | K | Joback Method |
| tc | 1208.64 | K | Joback Method |
| tf | 694.21 | K | Joback Method |
| vc | 0.755 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 476.97 | J/mol×K | 930.99 | Joback Method |
| cpg | 482.76 | J/mol×K | 977.26 | Joback Method |
| cpg | 487.73 | J/mol×K | 1023.54 | Joback Method |
| cpg | 491.95 | J/mol×K | 1069.81 | Joback Method |
| cpg | 495.51 | J/mol×K | 1116.09 | Joback Method |

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|---|---|---|---|---|
| cpg | 498.50 | J/mol×K | 1162.36 | Joback Method |
| cpg | 501.01 | J/mol×K | 1208.64 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373871&Units=SI |

# 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 |