# Benzoic acid, 3,5-dinitro, 2-methylpropyl ester

**Inchi:** InChI=1S/C11H12N2O6/c1-7(2)6-19-11(14)8-3-9(12(15)16)5-10(4-8)13(17)18/h3-5,7H,6
**InchiKey:** BIDNGDDDZYVORY-UHFFFAOYSA-N
**Formula:** C11H12N2O6
**SMILES:** CC(C)COC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 268.22
**CAS:** 10478-01-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -30.37 | kJ/mol | Joback Method |
| hf | -328.38 | kJ/mol | Joback Method |
| hfus | 39.49 | kJ/mol | Joback Method |
| hvap | 85.63 | kJ/mol | Joback Method |
| log10ws | -4.03 | | Crippen Method |
| logp | 2.316 | | Crippen Method |
| mcvol | 184.370 | ml/mol | McGowan Method |
| pc | 2784.72 | kPa | Joback Method |
| rinpol | 1897.00 | | NIST Webbook |
| rinpol | 1910.00 | | NIST Webbook |
| rinpol | 1983.00 | | NIST Webbook |
| rinpol | 1903.00 | | NIST Webbook |
| rinpol | 1889.00 | | NIST Webbook |
| rinpol | 1903.00 | | NIST Webbook |
| ripol | 2804.00 | | NIST Webbook |
| ripol | 2825.00 | | NIST Webbook |
| ripol | 2805.00 | | NIST Webbook |
| ripol | 2788.00 | | NIST Webbook |
| tb | 867.25 | K | Joback Method |
| tc | 1121.93 | K | Joback Method |
| tf | 609.57 | K | Joback Method |
| vc | 0.726 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 534.59 | J/mol×K | 867.25 | Joback Method |
| cpg | 544.76 | J/mol×K | 909.70 | Joback Method |
| cpg | 553.82 | J/mol×K | 952.14 | Joback Method |
| cpg | 561.80 | J/mol×K | 994.59 | Joback Method |
| cpg | 568.73 | J/mol×K | 1037.04 | Joback Method |
| cpg | 574.64 | J/mol×K | 1079.48 | Joback Method |
| cpg | 579.57 | J/mol×K | 1121.93 | Joback Method |

# Sources

**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=C10478010&Units=SI

# 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
**ripol:** Polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume