# Phthalic acid, 3,5-dinitro-4-methylbenzyl ethyl ester

**Inchi:** InChI=1S/C18H16N2O8/c1-3-27-17(21)13-6-4-5-7-14(13)18(22)28-10-12-8-15(19(23)24)
**InchiKey:** UMCIBIMLRJDHCU-UHFFFAOYSA-N
**Formula:** C18H16N2O8
**SMILES:** CCOC(=O)c1ccccc1C(=O)OCc1cc([N+](=O)[O-])c(C)c([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 388.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -109.76 | kJ/mol | Joback Method |
| hf | -498.79 | kJ/mol | Joback Method |
| hfus | 57.20 | kJ/mol | Joback Method |
| hvap | 114.36 | kJ/mol | Joback Method |
| log10ws | -6.26 | | Crippen Method |
| logp | 3.345 | | Crippen Method |
| mcvol | 266.680 | ml/mol | McGowan Method |
| pc | 2014.51 | kPa | Joback Method |
| rinpol | 3027.00 | | NIST Webbook |
| rinpol | 3027.00 | | NIST Webbook |
| tb | 1140.78 | K | Joback Method |
| tc | 1408.95 | K | Joback Method |
| tf | 827.08 | K | Joback Method |
| vc | 1.040 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 831.24 | J/mol×K | 1140.78 | Joback Method |
| cpg | 835.63 | J/mol×K | 1185.48 | Joback Method |
| cpg | 838.39 | J/mol×K | 1230.17 | Joback Method |
| cpg | 839.54 | J/mol×K | 1274.87 | Joback Method |
| cpg | 839.11 | J/mol×K | 1319.56 | Joback Method |
| cpg | 837.15 | J/mol×K | 1364.26 | Joback Method |
| cpg | 833.69 | J/mol×K | 1408.95 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415509&Units=SI |
| **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 |

# 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 |