# Phthalic acid, ethyl 3-methoxy-4-nitrobenzyl ester

**Inchi:** InChI=1S/C18H17NO7/c1-3-25-17(20)13-6-4-5-7-14(13)18(21)26-11-12-8-9-15(19(22)23
**InchiKey:** VWHBAXLHQKWNFW-UHFFFAOYSA-N
**Formula:** C18H17NO7
**SMILES:** CCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
**Mol. weight [g/mol]:** 359.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -240.68 | kJ/mol | Joback Method |
| hf | -608.78 | kJ/mol | Joback Method |
| hfus | 47.41 | kJ/mol | Joback Method |
| hvap | 99.51 | kJ/mol | Joback Method |
| log10ws | -5.26 | | Crippen Method |
| logp | 3.137 | | Crippen Method |
| mcvol | 255.130 | ml/mol | McGowan Method |
| pc | 1989.43 | kPa | Joback Method |
| rinpol | 3176.00 | | NIST Webbook |
| rinpol | 3176.00 | | NIST Webbook |
| tb | 1006.38 | K | Joback Method |
| tc | 1253.28 | K | Joback Method |
| tf | 693.18 | K | Joback Method |
| vc | 0.976 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 783.02 | J/mol×K | 1006.38 | Joback Method |
| cpg | 791.51 | J/mol×K | 1047.53 | Joback Method |
| cpg | 798.40 | J/mol×K | 1088.68 | Joback Method |
| cpg | 803.69 | J/mol×K | 1129.83 | Joback Method |
| cpg | 807.40 | J/mol×K | 1170.98 | Joback Method |
| cpg | 809.53 | J/mol×K | 1212.13 | Joback Method |
| cpg | 810.08 | J/mol×K | 1253.28 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382529&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 |