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

**Inchi:** InChI=1S/C22H25NO7/c1-3-4-5-8-13-29-21(24)17-9-6-7-10-18(17)22(25)30-15-16-11-12

**InchiKey:** FLZYRSJAXLMYOF-UHFFFAOYSA-N

**Formula:** C22H25NO7

**SMILES:** CCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])c(OC)c1

**Mol. weight [g/mol]:** 415.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -207.00 | kJ/mol | Joback Method |
| hf | -691.34 | kJ/mol | Joback Method |
| hfus | 57.77 | kJ/mol | Joback Method |
| hvap | 108.42 | kJ/mol | Joback Method |
| log10ws | -6.93 | | Crippen Method |
| logp | 4.697 | | Crippen Method |
| mcvol | 311.490 | ml/mol | McGowan Method |
| pc | 1450.14 | kPa | Joback Method |
| rinpol | 3685.00 | | NIST Webbook |
| rinpol | 3685.00 | | NIST Webbook |
| tb | 1097.90 | K | Joback Method |
| tc | 1347.03 | K | Joback Method |
| tf | 738.26 | K | Joback Method |
| vc | 1.200 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1013.99 | J/mol×K | 1097.90 | Joback Method |
| cpg | 1021.95 | J/mol×K | 1139.42 | Joback Method |
| cpg | 1028.11 | J/mol×K | 1180.94 | Joback Method |
| cpg | 1032.49 | J/mol×K | 1222.47 | Joback Method |
| cpg | 1035.12 | J/mol×K | 1263.99 | Joback Method |
| cpg | 1036.04 | J/mol×K | 1305.51 | Joback Method |
| cpg | 1035.26 | J/mol×K | 1347.03 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382534&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 |

# 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 |