# Terephthalic acid, 4-nitro-3-methylbenzyl pentyl ester

**Inchi:** InChI=1S/C21H23NO6/c1-3-4-5-12-27-20(23)17-7-9-18(10-8-17)21(24)28-14-16-6-11-19

**InchiKey:** FXNNYSBTYNAFCT-UHFFFAOYSA-N

**Formula:** C21H23NO6

**SMILES:** CCCCCOC(=O)c1ccc(C(=O)OCc2ccc([N+](=O)[O-])c(C)c2)cc1

**Mol. weight [g/mol]:** 385.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -110.42 | kJ/mol | Joback Method |
| hf | -538.48 | kJ/mol | Joback Method |
| hfus | 54.00 | kJ/mol | Joback Method |
| hvap | 103.78 | kJ/mol | Joback Method |
| log10ws | -6.87 | | Crippen Method |
| logp | 4.607 | | Crippen Method |
| mcvol | 291.530 | ml/mol | McGowan Method |
| pc | 1583.49 | kPa | Joback Method |
| rinpol | 3299.00 | | NIST Webbook |
| rinpol | 3299.00 | | NIST Webbook |
| tb | 1052.60 | K | Joback Method |
| tc | 1298.25 | K | Joback Method |
| tf | 704.76 | K | Joback Method |
| vc | 1.125 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 932.47 | J/mol×K | 1052.60 | Joback Method |
| cpg | 942.10 | J/mol×K | 1093.54 | Joback Method |
| cpg | 950.22 | J/mol×K | 1134.48 | Joback Method |
| cpg | 956.89 | J/mol×K | 1175.42 | Joback Method |
| cpg | 962.15 | J/mol×K | 1216.37 | Joback Method |
| cpg | 966.03 | J/mol×K | 1257.31 | Joback Method |
| cpg | 968.60 | J/mol×K | 1298.25 | Joback Method |

# Sources

| | |
|---|---|
| **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=U416102&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |