# Phthalic acid, butyl 2-(2-nitrophenyl)ethyl ester

**Inchi:** InChI=1S/C20H21NO6/c1-2-3-13-26-19(22)16-9-5-6-10-17(16)20(23)27-14-12-15-8-4-7-
**InchiKey:** MPEMNHVDPNTZMH-UHFFFAOYSA-N
**Formula:** C20H21NO6
**SMILES:** CCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 371.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -109.21 | kJ/mol | Joback Method |
| hf | -506.37 | kJ/mol | Joback Method |
| hfus | 51.79 | kJ/mol | Joback Method |
| hvap | 100.89 | kJ/mol | Joback Method |
| log10ws | -5.90 | | Crippen Method |
| logp | 3.951 | | Crippen Method |
| mcvol | 277.440 | ml/mol | McGowan Method |
| pc | 1733.22 | kPa | Joback Method |
| rinpol | 2848.00 | | NIST Webbook |
| rinpol | 2848.00 | | NIST Webbook |
| tb | 1024.74 | K | Joback Method |
| tc | 1269.43 | K | Joback Method |
| tf | 680.97 | K | Joback Method |
| vc | 1.069 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 875.97 | J/mol×K | 1024.74 | Joback Method |
| cpg | 885.81 | J/mol×K | 1065.52 | Joback Method |
| cpg | 894.23 | J/mol×K | 1106.30 | Joback Method |
| cpg | 901.28 | J/mol×K | 1147.09 | Joback Method |
| cpg | 907.01 | J/mol×K | 1187.87 | Joback Method |
| cpg | 911.45 | J/mol×K | 1228.65 | Joback Method |
| cpg | 914.67 | J/mol×K | 1269.43 | Joback Method |

# Sources

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|---|---|
| **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=U377994&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |