# bis-(4-Nitrophenyl)acetic acid, methyl ester

**Inchi:** InChI=1S/C15H12N2O6/c1-23-15(18)14(10-2-6-12(7-3-10)16(19)20)11-4-8-13(9-5-11)17
**InchiKey:** NNEDABBMQBFHAQ-UHFFFAOYSA-N
**Formula:** C15H12N2O6
**SMILES:** COC(=O)C(c1ccc([N+](=O)[O-])cc1)c1ccc([N+](=O)[O-])cc1
**Mol. weight [g/mol]:** 316.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 115.72 | kJ/mol | Joback Method |
| hf | -174.41 | kJ/mol | Joback Method |
| hfus | 43.90 | kJ/mol | Joback Method |
| hvap | 96.81 | kJ/mol | Joback Method |
| log10ws | -4.54 | | Crippen Method |
| logp | 2.808 | | Crippen Method |
| mcvol | 216.970 | ml/mol | McGowan Method |
| pc | 2635.25 | kPa | Joback Method |
| rinpol | 2676.00 | | NIST Webbook |
| rinpol | 2676.00 | | NIST Webbook |
| tb | 985.45 | K | Joback Method |
| tc | 1260.43 | K | Joback Method |
| tf | 681.07 | K | Joback Method |
| vc | 0.842 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 647.67 | J/mol×K | 985.45 | Joback Method |
| cpg | 656.37 | J/mol×K | 1031.28 | Joback Method |
| cpg | 663.79 | J/mol×K | 1077.11 | Joback Method |
| cpg | 670.00 | J/mol×K | 1122.94 | Joback Method |
| cpg | 675.09 | J/mol×K | 1168.77 | Joback Method |
| cpg | 679.15 | J/mol×K | 1214.60 | Joback Method |
| cpg | 682.25 | J/mol×K | 1260.43 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R190060&Units=SI |

# 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 |