# (Z)-3-(p-Methylphenylamino)-2-nitrocrotonic acid methyl ester

**Inchi:** InChI=1S/C12H14N2O4/c1-8-4-6-10(7-5-8)13-9(2)11(14(16)17)12(15)18-3/h4-7,13H,1-3

**InchiKey:** CPKKJRLGHKIKRG-LUAWRHEFSA-N

**Formula:** C12H14N2O4

**SMILES:** COC(=O)C(=C(C)Nc1ccc(C)cc1)[N+](=O)[O-]

**Mol. weight [g/mol]:** 250.25

**CAS:** 116343-85-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 107.08 | kJ/mol | Joback Method |
| hf | -170.40 | kJ/mol | Joback Method |
| hfus | 37.32 | kJ/mol | Joback Method |
| hvap | 77.55 | kJ/mol | Joback Method |
| log10ws | -3.42 | | Crippen Method |
| logp | 2.088 | | Crippen Method |
| mcvol | 186.720 | ml/mol | McGowan Method |
| pc | 2709.85 | kPa | Joback Method |
| tb | 787.84 | K | Joback Method |
| tc | 1029.73 | K | Joback Method |
| tf | 499.37 | K | Joback Method |
| vc | 0.723 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 521.97 | J/mol×K | 787.84 | Joback Method |
| cpg | 534.30 | J/mol×K | 828.15 | Joback Method |
| cpg | 545.63 | J/mol×K | 868.47 | Joback Method |
| cpg | 556.02 | J/mol×K | 908.78 | Joback Method |
| cpg | 565.53 | J/mol×K | 949.10 | Joback Method |
| cpg | 574.22 | J/mol×K | 989.41 | Joback Method |
| cpg | 582.14 | J/mol×K | 1029.73 | Joback Method |

# Sources

| | |
|---|---|
| **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=C116343852&Units=SI |

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