# M-nitro cinnamic acid, methyl ester

**Inchi:** InChI=1S/C10H9NO4/c1-15-10(12)6-5-8-3-2-4-9(7-8)11(13)14/h2-7H,1H3/b6-5+
**InchiKey:** DKQXESBKFCYESZ-AATRIKPKSA-N
**Formula:** C10H9NO4
**SMILES:** COC(=O)C=Cc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 207.18
**CAS:** 1664-59-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 17.95 | kJ/mol | Joback Method |
| hf | -163.01 | kJ/mol | Joback Method |
| hfus | 29.66 | kJ/mol | Joback Method |
| hvap | 66.50 | kJ/mol | Joback Method |
| log10ws | -2.65 | | Crippen Method |
| logp | 1.781 | | Crippen Method |
| mcvol | 148.560 | ml/mol | McGowan Method |
| pc | 3257.86 | kPa | Joback Method |
| tb | 692.15 | K | Joback Method |
| tc | 939.29 | K | Joback Method |
| tf | 452.09 | K | Joback Method |
| vc | 0.574 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 371.69 | J/mol×K | 692.15 | Joback Method |
| cpg | 383.11 | J/mol×K | 733.34 | Joback Method |
| cpg | 393.60 | J/mol×K | 774.53 | Joback Method |
| cpg | 403.23 | J/mol×K | 815.72 | Joback Method |
| cpg | 412.03 | J/mol×K | 856.91 | Joback Method |
| cpg | 420.05 | J/mol×K | 898.10 | Joback Method |
| cpg | 427.33 | J/mol×K | 939.29 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1664591&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

| | |
|---|---|
| **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 |

Latest version available from:
https://www.chemeo.com/cid/93-305-0/M-nitro-cinnamic-acid-methyl-ester.pdf
Generated by Cheméo on 2024-04-25 06:49:11.223090601 +0000 UTC m=+16317000.143667925.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.