# Fumaric acid, ethyl 3-nitrophenyl ester

**Inchi:** InChI=1S/C12H11NO6/c1-2-18-11(14)6-7-12(15)19-10-5-3-4-9(8-10)13(16)17/h3-8H,2H2
**InchiKey:** FLMSXPCTJTUQGF-VOTSOKGWSA-N
**Formula:** C12H11NO6
**SMILES:** CCOC(=O)C=CC(=O)Oc1cccc([N+](=O)[O-])c1
**Mol. weight [g/mol]:** 265.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -199.13 | kJ/mol | Joback Method |
| hf | -449.09 | kJ/mol | Joback Method |
| hfus | 37.62 | kJ/mol | Joback Method |
| hvap | 80.10 | kJ/mol | Joback Method |
| log10ws | -2.83 | | Crippen Method |
| logp | 1.619 | | Crippen Method |
| mcvol | 184.180 | ml/mol | McGowan Method |
| pc | 2775.92 | kPa | Joback Method |
| rinpol | 2224.00 | | NIST Webbook |
| rinpol | 2224.00 | | NIST Webbook |
| tb | 814.20 | K | Joback Method |
| tc | 1053.13 | K | Joback Method |
| tf | 546.79 | K | Joback Method |
| vc | 0.710 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 506.62 | J/mol×K | 814.20 | Joback Method |
| cpg | 517.16 | J/mol×K | 854.02 | Joback Method |
| cpg | 526.71 | J/mol×K | 893.84 | Joback Method |
| cpg | 535.30 | J/mol×K | 933.66 | Joback Method |
| cpg | 542.95 | J/mol×K | 973.49 | Joback Method |
| cpg | 549.70 | J/mol×K | 1013.31 | Joback Method |
| cpg | 555.56 | J/mol×K | 1053.13 | 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=U348185&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 |