# Formic acid, (4-methyl-3-nitrophenyl)methyl ester

**Inchi:** InChI=1S/C9H9NO4/c1-7-2-3-8(5-14-6-11)4-9(7)10(12)13/h2-4,6H,5H2,1H3
**InchiKey:** ORFBBOBPAWUFAS-UHFFFAOYSA-N
**Formula:** C9H9NO4
**SMILES:** Cc1ccc(COC=O)cc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 195.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -50.92 | kJ/mol | Joback Method |
| hf | -244.06 | kJ/mol | Joback Method |
| hfus | 27.17 | kJ/mol | Joback Method |
| hvap | 64.95 | kJ/mol | Joback Method |
| log10ws | -2.76 | | Crippen Method |
| logp | 1.576 | | Crippen Method |
| mcvol | 138.770 | ml/mol | McGowan Method |
| pc | 3411.87 | kPa | Joback Method |
| rinpol | 1610.00 | | NIST Webbook |
| tb | 664.88 | K | Joback Method |
| tc | 902.91 | K | Joback Method |
| tf | 450.49 | K | Joback Method |
| vc | 0.548 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 345.52 | J/mol×K | 664.88 | Joback Method |
| cpg | 356.53 | J/mol×K | 704.55 | Joback Method |
| cpg | 366.74 | J/mol×K | 744.22 | Joback Method |
| cpg | 376.18 | J/mol×K | 783.89 | Joback Method |
| cpg | 384.86 | J/mol×K | 823.56 | Joback Method |
| cpg | 392.79 | J/mol×K | 863.24 | Joback Method |
| cpg | 399.98 | J/mol×K | 902.91 | 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=U368226&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 |

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