# m-Anisic acid, 3,5-dimethylphenyl ester

**Inchi:** InChI=1S/C16H16O3/c1-11-7-12(2)9-15(8-11)19-16(17)13-5-4-6-14(10-13)18-3/h4-10H,1
**InchiKey:** WBMONHGBQBMFNO-UHFFFAOYSA-N
**Formula:** C16H16O3
**SMILES:** COc1cccc(C(=O)Oc2cc(C)cc(C)c2)c1
**Mol. weight [g/mol]:** 256.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -59.15 | kJ/mol | Joback Method |
| hf | -311.94 | kJ/mol | Joback Method |
| hfus | 28.09 | kJ/mol | Joback Method |
| hvap | 69.31 | kJ/mol | Joback Method |
| log10ws | -4.63 | | Crippen Method |
| logp | 3.531 | | Crippen Method |
| mcvol | 202.090 | ml/mol | McGowan Method |
| pc | 2250.40 | kPa | Joback Method |
| rinpol | 2088.00 | | NIST Webbook |
| rinpol | 2088.00 | | NIST Webbook |
| tb | 732.49 | K | Joback Method |
| tc | 964.63 | K | Joback Method |
| tf | 454.87 | K | Joback Method |
| vc | 0.757 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 542.39 | J/mol×K | 732.49 | Joback Method |
| cpg | 557.61 | J/mol×K | 771.18 | Joback Method |
| cpg | 571.68 | J/mol×K | 809.87 | Joback Method |
| cpg | 584.61 | J/mol×K | 848.56 | Joback Method |
| cpg | 596.44 | J/mol×K | 887.25 | Joback Method |
| cpg | 607.15 | J/mol×K | 925.94 | Joback Method |
| cpg | 616.78 | J/mol×K | 964.63 | Joback Method |
| dvisc | 0.0006069 | Pa×s | 454.87 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003867 | Pa×s | 501.14 | Joback Method |
| dvisc | 0.0002659 | Pa×s | 547.41 | Joback Method |
| dvisc | 0.0001938 | Pa×s | 593.68 | Joback Method |
| dvisc | 0.0001479 | Pa×s | 639.95 | Joback Method |
| dvisc | 0.0001171 | Pa×s | 686.22 | Joback Method |
| dvisc | 0.0000954 | Pa×s | 732.49 | 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=U307800&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |