# 4-Methoxybenzene-1,3-diamine, N1,N1,N3-triacetyl-

**Inchi:** InChI=1S/C13H16N2O4/c1-8(16)14-12-7-11(5-6-13(12)19-4)15(9(2)17)10(3)18/h5-7H,1-

**InchiKey:** DQPHCEHTPHJVPY-UHFFFAOYSA-N

**Formula:** C13H16N2O4

**SMILES:** COc1ccc(N(C(C)=O)C(C)=O)cc1NC(C)=O

**Mol. weight [g/mol]:** 264.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -139.86 | kJ/mol | Joback Method |
| hf | -447.02 | kJ/mol | Joback Method |
| hfus | 36.79 | kJ/mol | Joback Method |
| hvap | 79.26 | kJ/mol | Joback Method |
| log10ws | -2.09 | | Crippen Method |
| logp | 1.553 | | Crippen Method |
| mcvol | 200.810 | ml/mol | McGowan Method |
| pc | 2545.61 | kPa | Joback Method |
| rinpol | 2258.00 | | NIST Webbook |
| tb | 780.12 | K | Joback Method |
| tc | 995.18 | K | Joback Method |
| tf | 544.88 | K | Joback Method |
| vc | 0.745 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 565.53 | J/mol×K | 780.12 | Joback Method |
| cpg | 577.70 | J/mol×K | 815.96 | Joback Method |
| cpg | 588.93 | J/mol×K | 851.81 | Joback Method |
| cpg | 599.24 | J/mol×K | 887.65 | Joback Method |
| cpg | 608.66 | J/mol×K | 923.49 | Joback Method |
| cpg | 617.21 | J/mol×K | 959.33 | Joback Method |
| cpg | 624.91 | J/mol×K | 995.18 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373209&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

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