

4-Methoxy-o-phenylenediamine

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| Other names: | 4-Methoxy-1,2-diaminobenzene o-Phenylenediamine, 4-methoxy- 1,2-Benzenediamine, 4-methoxy- 3,4-Diaminoanisole |
| Inchi: | InChI=1S/C7H10N2O/c1-10-5-2-3-6(8)7(9)4-5/h2-4H,8-9H2,1H3 |
| InchiKey: | AGAHETWGCFCMDK-UHFFFAOYSA-N |
| Formula: | C7H10N2O |
| SMILES: | COc1ccc(N)c(N)c1 |
| Mol. weight [g/mol]: | 138.17 |
| CAS: | 102-51-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 129.11 | kJ/mol | Joback Method |
| hf | -38.86 | kJ/mol | Joback Method |
| hfus | 18.73 | kJ/mol | Joback Method |
| hvap | 58.47 | kJ/mol | Joback Method |
| log10ws | -0.86 | | Crippen Method |
| logp | 0.860 | | Crippen Method |
| mcvol | 111.560 | ml/mol | McGowan Method |
| pc | 4492.23 | kPa | Joback Method |
| tb | 563.68 | K | Joback Method |
| tc | 800.40 | K | Joback Method |
| tf | 408.86 | K | Joback Method |
| vc | 0.396 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 258.94 | J/molxK | 563.68 | Joback Method |
| cpg | 269.93 | J/molxK | 603.13 | Joback Method |
| cpg | 280.29 | J/molxK | 642.59 | Joback Method |
| cpg | 290.02 | J/molxK | 682.04 | Joback Method |
| cpg | 299.14 | J/molxK | 721.49 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 307.64 | J/mol×K | 760.95 | Joback Method |
| cpg | 315.52 | J/mol×K | 800.40 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C102512&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 |

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