

# Benzene, 1,4-dichloro-2-methoxy-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2,5-Dichloroanizole<br>1,4-Dichloro-2-methoxybenzene<br>2,5-Dichlorophenol, methyl ether<br>2,5-Dichloroanisole |
| <b>Inchi:</b>               | InChI=1S/C7H6Cl2O/c1-10-7-4-5(8)2-3-6(7)9/h2-4H,1H3   |
| <b>InchiKey:</b>            | QKMNFFSBZRGHDJ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C7H6Cl2O  |
| <b>SMILES:</b>              | COc1cc(Cl)ccc1Cl  |
| <b>Mol. weight [g/mol]:</b> | 177.03  |
| <b>CAS:</b>                 | 1984-58-3   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -27.65  | kJ/mol | Joback Method  |
| hf            | -137.92 | kJ/mol | Joback Method  |
| hfus          | 16.73   | kJ/mol | Joback Method  |
| hvap          | 45.96   | kJ/mol | Joback Method  |
| log10ws       | -2.96   |        | Crippen Method |
| logp          | 3.002   |        | Crippen Method |
| mcvol         | 116.080 | ml/mol | McGowan Method |
| pc            | 3543.08 | kPa    | Joback Method  |
| rinpol        | 1260.00 |        | NIST Webbook   |
| rinpol        | 1293.90 |        | NIST Webbook   |
| rinpol        | 1241.00 |        | NIST Webbook   |
| rinpol        | 1239.00 |        | NIST Webbook   |
| rinpol        | 1241.00 |        | NIST Webbook   |
| rinpol        | 1254.00 |        | NIST Webbook   |
| rinpol        | 1293.90 |        | NIST Webbook   |
| rinpol        | 1273.00 |        | NIST Webbook   |
| rinpol        | 1256.00 |        | NIST Webbook   |
| rinpol        | 1244.00 |        | NIST Webbook   |
| rinpol        | 1260.00 |        | NIST Webbook   |
| rinpol        | 1264.00 |        | NIST Webbook   |
| ripol         | 1886.00 |        | NIST Webbook   |
| ripol         | 1857.00 |        | NIST Webbook   |
| ripol         | 1857.00 |        | NIST Webbook   |
| ripol         | 1845.00 |        | NIST Webbook   |

|       |         |                      |               |
|-------|---------|----------------------|---------------|
| ripol | 1857.00 |                      | NIST Webbook  |
| ripol | 1892.00 |                      | NIST Webbook  |
| ripol | 1874.00 |                      | NIST Webbook  |
| tb    | 493.48  | K                    | Joback Method |
| tc    | 720.45  | K                    | Joback Method |
| tf    | 302.18  | K                    | Joback Method |
| vc    | 0.435   | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 206.95    | J/molxK | 493.48          | Joback Method |
| cpg           | 216.08    | J/molxK | 531.31          | Joback Method |
| cpg           | 224.74    | J/molxK | 569.14          | Joback Method |
| cpg           | 232.93    | J/molxK | 606.96          | Joback Method |
| cpg           | 240.65    | J/molxK | 644.79          | Joback Method |
| cpg           | 247.90    | J/molxK | 682.62          | Joback Method |
| cpg           | 254.69    | J/molxK | 720.45          | Joback Method |
| dvisc         | 0.0013457 | Paxs    | 302.18          | Joback Method |
| dvisc         | 0.0008743 | Paxs    | 334.06          | Joback Method |
| dvisc         | 0.0006124 | Paxs    | 365.95          | Joback Method |
| dvisc         | 0.0004541 | Paxs    | 397.83          | Joback Method |
| dvisc         | 0.0003521 | Paxs    | 429.71          | Joback Method |
| dvisc         | 0.0002827 | Paxs    | 461.60          | Joback Method |
| dvisc         | 0.0002335 | Paxs    | 493.48          | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 413.20 | K    | 5.30           | NIST Webbook |

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Joback Method:

[https://en.wikipedia.org/wiki/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=C1984583&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  
**ripol:** Polar retention indices  
**tb:** Normal Boiling Point Temperature  
**tbrp:** Boiling point at reduced pressure  
**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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