# Benzene, 1-(chloromethyl)-3-methoxy-

| | |
|---|---|
| **Other names:** | Anisole, m-(chloromethyl)- |
| | m-(Chloromethyl)anisole |
| | m-Methoxybenzyl chloride |
| | Toluene, «alpha»-chloro-m-methocy- |
| | 1-(Chloromethyl)-3-methoxybenzene |
| | 3-Methoxybenzyl chloride |
| | «alpha»-Chloro-3-methoxytoluene |
| **Inchi:** | InChI=1S/C8H9ClO/c1-10-8-4-2-3-7(5-8)6-9/h2-5H,6H2,1H3 |
| **InchiKey:** | VGISFWWEOGVMED-UHFFFAOYSA-N |
| **Formula:** | C8H9ClO |
| **SMILES:** | COc1cccc(CCl)c1 |
| **Mol. weight [g/mol]:** | 156.61 |
| **CAS:** | 824-98-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 2.33 | kJ/mol | Joback Method |
| hf | -131.35 | kJ/mol | Joback Method |
| hfus | 15.51 | kJ/mol | Joback Method |
| hvap | 43.14 | kJ/mol | Joback Method |
| log10ws | -2.62 | | Crippen Method |
| logp | 2.434 | | Crippen Method |
| mcvol | 117.930 | ml/mol | McGowan Method |
| pc | 3364.54 | kPa | Joback Method |
| tb | 473.95 | K | Joback Method |
| tc | 690.26 | K | Joback Method |
| tf | 271.01 | K | Joback Method |
| vc | 0.443 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 224.21 | J/mol×K | 473.95 | Joback Method |
| cpg | 275.56 | J/mol×K | 654.20 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 266.42 | J/mol×K | 618.15 | Joback Method |
| cpg | 256.73 | J/mol×K | 582.10 | Joback Method |
| cpg | 246.47 | J/mol×K | 546.05 | Joback Method |
| cpg | 235.63 | J/mol×K | 510.00 | Joback Method |
| cpg | 284.16 | J/mol×K | 690.26 | Joback Method |
| dvisc | 0.0002194 | Pa×s | 473.95 | Joback Method |
| dvisc | 0.0002727 | Pa×s | 440.13 | Joback Method |
| dvisc | 0.0003513 | Pa×s | 406.30 | Joback Method |
| dvisc | 0.0004738 | Pa×s | 372.48 | Joback Method |
| dvisc | 0.0006786 | Pa×s | 338.66 | Joback Method |
| dvisc | 0.0010524 | Pa×s | 304.83 | Joback Method |
| dvisc | 0.0018210 | Pa×s | 271.01 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 397.20 | K | 1.70 | NIST Webbook |

# Sources

**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=C824986&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |