# 3,4-(Methylenedioxy)toluene

| | |
|---|---|
| **Other names:** | 1,3-Benzodioxole, 5-methyl- |
| | 5-methyl-1,3-benzodioxole |
| **Inchi:** | InChI=1S/C8H8O2/c1-6-2-3-7-8(4-6)10-5-9-7/h2-4H,5H2,1H3 |
| **InchiKey:** | GHPODDMCSOYWNE-UHFFFAOYSA-N |
| **Formula:** | C8H8O2 |
| **SMILES:** | Cc1ccc2c(c1)OCO2 |
| **Mol. weight [g/mol]:** | 136.15 |
| **CAS:** | 7145-99-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 5.85 | kJ/mol | Joback Method |
| hf | -165.72 | kJ/mol | Joback Method |
| hfus | 22.76 | kJ/mol | Joback Method |
| hvap | 54.90 ± 1.20 | kJ/mol | NIST Webbook |
| log10ws | -2.16 | | Crippen Method |
| logp | 1.724 | | Crippen Method |
| mcvol | 100.700 | ml/mol | McGowan Method |
| pc | 4216.56 | kPa | Joback Method |
| tb | 472.70 | K | NIST Webbook |
| tc | 713.45 | K | Joback Method |
| tf | 306.70 | K | Joback Method |
| vc | 0.376 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 214.69 | J/mol×K | 484.39 | Joback Method |
| cpg | 226.38 | J/mol×K | 522.57 | Joback Method |
| cpg | 237.23 | J/mol×K | 560.74 | Joback Method |
| cpg | 247.29 | J/mol×K | 598.92 | Joback Method |
| cpg | 256.62 | J/mol×K | 637.10 | Joback Method |
| cpg | 265.27 | J/mol×K | 675.27 | Joback Method |
| cpg | 273.30 | J/mol×K | 713.45 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0019633 | Pa×s | 306.70 | Joback Method |
| dvisc | 0.0013990 | Pa×s | 336.31 | Joback Method |
| dvisc | 0.0010531 | Pa×s | 365.93 | Joback Method |
| dvisc | 0.0008272 | Pa×s | 395.54 | Joback Method |
| dvisc | 0.0006720 | Pa×s | 425.16 | Joback Method |
| dvisc | 0.0005608 | Pa×s | 454.77 | Joback Method |
| dvisc | 0.0004785 | Pa×s | 484.39 | Joback Method |
| hvapt | 54.90 | kJ/mol | 298.15 | Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 352.00 ± 1.00 | K | 1.90 | NIST Webbook |

# Sources

| | |
|---|---|
| **Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives:** | https://www.doi.org/10.1021/je700035m |
| **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=C7145995&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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |

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

Latest version available from:

https://www.chemeo.com/cid/35-560-1/3-4-Methylenedioxy-toluene.pdf

Generated by Cheméo on 2024-04-20 04:39:26.19657341 +0000 UTC m=+15877215.117150722.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.