

Benzene, 1,2-dichloro-4,5-dimethoxy-

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|-----------------------------|--|
| Other names: | 1,2-Dimethoxy-4,5-dichloro-benzene 4,5-Dichloroveratrole Benzene, 4,5-dichloro-1,2-dimethoxy |
| Inchi: | InChI=1S/C8H8Cl2O2/c1-11-7-3-5(9)6(10)4-8(7)12-2/h3-4H,1-2H3 |
| InchiKey: | RJYXLZQZBLGBOM-UHFFFAOYSA-N |
| Formula: | C8H8Cl2O2 |
| SMILES: | COc1cc(Cl)c(Cl)cc1OC |
| Mol. weight [g/mol]: | 207.05 |
| CAS: | 2772-46-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|--------------------------------------|
| gf | -133.86 | kJ/mol | Joback Method |
| hf | -302.25 | kJ/mol | Joback Method |
| hfus | 20.12 | kJ/mol | Joback Method |
| hvap | 51.25 | kJ/mol | Joback Method |
| log10ws | -3.46 | | Aqueous Solubility Prediction Method |
| logp | 3.011 | | Crippen Method |
| mcvol | 136.040 | ml/mol | McGowan Method |
| pc | 3059.17 | kPa | Joback Method |
| rinpol | 1503.00 | | NIST Webbook |
| rinpol | 1497.00 | | NIST Webbook |
| rinpol | 1484.00 | | NIST Webbook |
| rinpol | 1483.00 | | NIST Webbook |
| rinpol | 1484.00 | | NIST Webbook |
| rinpol | 1484.00 | | NIST Webbook |
| ripol | 2188.00 | | NIST Webbook |
| ripol | 2216.00 | | NIST Webbook |
| ripol | 2228.00 | | NIST Webbook |
| ripol | 2213.00 | | NIST Webbook |
| ripol | 2203.00 | | NIST Webbook |
| tb | 543.76 | K | Joback Method |
| tc | 765.36 | K | Joback Method |
| tf | 348.20 | K | Joback Method |
| vc | 0.509 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 268.48 | J/molxK | 543.76 | Joback Method |
| cpg | 278.53 | J/molxK | 580.69 | Joback Method |
| cpg | 288.14 | J/molxK | 617.63 | Joback Method |
| cpg | 297.29 | J/molxK | 654.56 | Joback Method |
| cpg | 305.98 | J/molxK | 691.49 | Joback Method |
| cpg | 314.19 | J/molxK | 728.42 | Joback Method |
| cpg | 321.89 | J/molxK | 765.36 | Joback Method |
| dvisc | 0.0008515 | Paxs | 348.20 | Joback Method |
| dvisc | 0.0005846 | Paxs | 380.79 | Joback Method |
| dvisc | 0.0004258 | Paxs | 413.39 | Joback Method |
| dvisc | 0.0003249 | Paxs | 445.98 | Joback Method |
| dvisc | 0.0002572 | Paxs | 478.57 | Joback Method |
| dvisc | 0.0002098 | Paxs | 511.17 | Joback Method |
| dvisc | 0.0001753 | Paxs | 543.76 | Joback Method |

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2772465&Units=SI>

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

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|-----------------|-------------------------------------|
| 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 |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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