# Apiol

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|---|---|
| **Other names:** | 1,3-Benzodioxole, 4,7-dimethoxy-5-(2-propenyl)- |
| | Benzene, 1-allyl-2,5-dimethoxy-3,4-(methylenedioxy)- |
| | Apiole |
| | Apioline |
| | Parsley apiole |
| | Parsley camphor |
| | 1-Allyl-2,5-dimethoxy-3,4-(methylenedioxy)benzene |
| | 4,7-Dimethoxy-5-(2-propenyl)-1,3-benzodioxole |
| | 1,3-Benzodioxole, 4,7-dimethoxy-5-(2-propen-1-yl)- |
| | NSC 9070 |
| | 5-allyl-4,7-dimethoxy-1,3-benzodioxole |
| | 4,7-Dimethoxy-5-(2-propen-1-yl)-1,3-benzodioxole (apiol) |
| **Inchi:** | InChI=1S/C12H14O4/c1-4-5-8-6-9(13-2)11-12(10(8)14-3)16-7-15-11/h4,6H,1,5,7H2,2-3H |
| **InchiKey:** | QQRSPHJOOXUALR-UHFFFAOYSA-N |
| **Formula:** | C12H14O4 |
| **SMILES:** | C=CCc1cc(OC)c2c(c1OC)OCO2 |
| **Mol. weight [g/mol]:** | 222.24 |
| **CAS:** | 523-80-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -101.89 | kJ/mol | Joback Method |
| hf | -410.23 | kJ/mol | Joback Method |
| hfus | 33.44 | kJ/mol | Joback Method |
| hvap | 60.62 | kJ/mol | Joback Method |
| log10ws | -3.00 | | Crippen Method |
| logp | 2.161 | | Crippen Method |
| mcvol | 164.500 | ml/mol | McGowan Method |
| pc | 2640.67 | kPa | Joback Method |
| rinpol | 1679.00 | | NIST Webbook |
| rinpol | 1674.00 | | NIST Webbook |
| rinpol | 1687.00 | | NIST Webbook |
| rinpol | 1685.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1681.00 | | NIST Webbook |
| rinpol | 1691.00 | | NIST Webbook |

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| rinpol | 1687.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1681.00 | | NIST Webbook |
| rinpol | 1651.00 | | NIST Webbook |
| rinpol | 1689.00 | | NIST Webbook |
| rinpol | 1691.00 | | NIST Webbook |
| rinpol | 1645.00 | | NIST Webbook |
| rinpol | 1642.00 | | NIST Webbook |
| rinpol | 1687.00 | | NIST Webbook |
| rinpol | 1675.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1696.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1671.00 | | NIST Webbook |
| rinpol | 1676.00 | | NIST Webbook |
| rinpol | 1679.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1682.00 | | NIST Webbook |
| rinpol | 1681.00 | | NIST Webbook |
| rinpol | 1676.00 | | NIST Webbook |
| rinpol | 1651.00 | | NIST Webbook |
| ripol | 2431.00 | | NIST Webbook |
| ripol | 2460.00 | | NIST Webbook |
| ripol | 2431.00 | | NIST Webbook |
| tb | 627.39 | K | Joback Method |
| tc | 842.34 | K | Joback Method |
| tf | 302.40 ± 0.05 | K | NIST Webbook |
| vc | 0.617 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 491.71 | J/mol×K | 842.34 | Joback Method |
| cpg | 421.38 | J/mol×K | 627.39 | Joback Method |
| cpg | 434.89 | J/mol×K | 663.21 | Joback Method |
| cpg | 447.67 | J/mol×K | 699.04 | Joback Method |
| cpg | 459.71 | J/mol×K | 734.86 | Joback Method |
| cpg | 471.05 | J/mol×K | 770.69 | Joback Method |
| cpg | 481.71 | J/mol×K | 806.51 | Joback Method |
| dvisc | 0.0002663 | Pa×s | 627.39 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0009674 | Pa×s | 419.52 | Joback Method |
| dvisc | 0.0007188 | Pa×s | 454.17 | Joback Method |
| dvisc | 0.0005571 | Pa×s | 488.81 | Joback Method |
| dvisc | 0.0004466 | Pa×s | 523.46 | Joback Method |
| dvisc | 0.0003679 | Pa×s | 558.10 | Joback Method |
| dvisc | 0.0003101 | Pa×s | 592.75 | Joback Method |
| hvapt | 70.60 | kJ/mol | 473.50 | NIST Webbook |

# Sources

**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
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C523808&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
**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
**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