# 1,3-Benzodioxole, 5-(1-propenyl)-

| | |
|---|---|
| **Other names:** | Benzene, 1,2-(methylenedioxy)-4-propenyl- |
| | Isosafrole |
| | Izosafrol |
| | 1,2-(Methylenedioxy)-4-propenylbenzene |
| | 3,4-(Methylenedioxy)-1-propenylbenzene |
| | 4-Propenyl-1,2-methylenedioxybenzene |
| | 4-Propenylcatechol methylene ether |
| | 5-(1-Propenyl)-1,3-benzodioxole |
| | Rcra waste number U141 |
| | Isosafrol |
| | 1,3-Benzodioxole, 5-(1-propen-1-yl)- |
| | 6-(1-Propenyl)-1,3-benzodioxole |
| | NSC 4884 |
| | 5-prop-1-enyl-1,3-benzodioxole |
| **Inchi:** | InChI=1S/C10H10O2/c1-2-3-8-4-5-9-10(6-8)12-7-11-9/h2-6H,7H2,1H3 |
| **InchiKey:** | VHVOLFRBFDOUSH-UHFFFAOYSA-N |
| **Formula:** | C10H10O2 |
| **SMILES:** | CC=Cc1ccc2c(c1)OCO2 |
| **Mol. weight [g/mol]:** | 162.19 |
| **CAS:** | 120-58-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 102.91 | kJ/mol | Joback Method |
| hf | -89.78 | kJ/mol | Joback Method |
| hfus | 28.14 | kJ/mol | Joback Method |
| hvap | 50.65 | kJ/mol | Joback Method |
| log10ws | -2.92 | | Crippen Method |
| logp | 2.448 | | Crippen Method |
| mcvol | 124.580 | ml/mol | McGowan Method |
| pc | 3543.08 | kPa | Joback Method |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1298.00 | | NIST Webbook |
| rinpol | 234.79 | | NIST Webbook |
| rinpol | 235.68 | | NIST Webbook |
| rinpol | 1360.00 | | NIST Webbook |
| rinpol | 1296.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| rinpol | 1296.00 | | NIST Webbook |
| rinpol | 1355.00 | | NIST Webbook |
| rinpol | 1357.00 | | NIST Webbook |
| ripol | 2029.00 | | NIST Webbook |
| ripol | 2029.00 | | NIST Webbook |
| ripol | 2040.00 | | NIST Webbook |
| tb | 534.31 | K | Joback Method |
| tc | 766.11 | K | Joback Method |
| tf | 324.16 | K | Joback Method |
| vc | 0.468 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 347.33 | J/mol×K | 766.11 | Joback Method |
| cpg | 338.36 | J/mol×K | 727.47 | Joback Method |
| cpg | 328.73 | J/mol×K | 688.84 | Joback Method |
| cpg | 318.35 | J/mol×K | 650.21 | Joback Method |
| cpg | 307.14 | J/mol×K | 611.58 | Joback Method |
| cpg | 295.01 | J/mol×K | 572.94 | Joback Method |
| cpg | 281.89 | J/mol×K | 534.31 | Joback Method |
| dvisc | 0.0019464 | Pa×s | 324.16 | Joback Method |
| dvisc | 0.0003807 | Pa×s | 534.31 | Joback Method |
| dvisc | 0.0004543 | Pa×s | 499.28 | Joback Method |
| dvisc | 0.0005566 | Pa×s | 464.26 | Joback Method |
| dvisc | 0.0007050 | Pa×s | 429.24 | Joback Method |
| dvisc | 0.0009313 | Pa×s | 394.21 | Joback Method |
| dvisc | 0.0012988 | Pa×s | 359.19 | Joback Method |
| hvapt | 59.40 | kJ/mol | 462.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 354.70 | K | 0.50 | 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=C120581&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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |