# Isoeugenol, benzyl ether

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|---|---|
| **Other names:** | Benzene, 2-methoxy-1-(phenylmethoxy)-4-(1-propenyl)- |
| | Benzene, 1-(benzyloxy)-2-methoxy-4-propenyl- |
| | Benzyl alcohol, ether with isoeugenol |
| | Benzyl isoeugenol |
| | Benzyl isoeugenol ether |
| | Benzyl 2-methoxy-4-propenylphenyl ether |
| | 1-(Benzyloxy)-2-methoxy-4-(1-propenyl)benzene |
| | Benzene, 2-methoxy-1-(phenylmethoxy)-4-(1-propen-1-yl)- |
| | NSC 46157 |
| | benzyl 2-methoxy-4-prop-1-enylphenyl ether |
| **Inchi:** | InChI=1S/C17H18O2/c1-3-7-14-10-11-16(17(12-14)18-2)19-13-15-8-5-4-6-9-15/h3-12H,1 |
| **InchiKey:** | YKSSSKBJDZDZTD-XVNBXDOJSA-N |
| **Formula:** | C17H18O2 |
| **SMILES:** | CC=Cc1ccc(OCc2ccccc2)c(OC)c1 |
| **Mol. weight [g/mol]:** | 254.32 |
| **CAS:** | 120-11-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 168.04 | kJ/mol | Joback Method |
| hf | -91.31 | kJ/mol | Joback Method |
| hfus | 29.67 | kJ/mol | Joback Method |
| hvap | 64.09 | kJ/mol | Joback Method |
| log10ws | -5.06 | | Crippen Method |
| logp | 4.307 | | Crippen Method |
| mcvol | 210.310 | ml/mol | McGowan Method |
| pc | 2066.12 | kPa | Joback Method |
| rinpol | 2078.40 | | NIST Webbook |
| rinpol | 2078.40 | | NIST Webbook |
| tb | 700.68 | K | Joback Method |
| tc | 930.89 | K | Joback Method |
| tf | 398.61 | K | Joback Method |
| vc | 0.787 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 556.28 | J/mol×K | 700.68 | Joback Method |
| cpg | 573.27 | J/mol×K | 739.05 | Joback Method |
| cpg | 589.08 | J/mol×K | 777.42 | Joback Method |
| cpg | 603.75 | J/mol×K | 815.79 | Joback Method |
| cpg | 617.32 | J/mol×K | 854.16 | Joback Method |
| cpg | 629.83 | J/mol×K | 892.52 | Joback Method |
| cpg | 641.34 | J/mol×K | 930.89 | Joback Method |
| dvisc | 0.0006987 | Pa×s | 398.61 | Joback Method |
| dvisc | 0.0003874 | Pa×s | 448.96 | Joback Method |
| dvisc | 0.0002420 | Pa×s | 499.30 | Joback Method |
| dvisc | 0.0001647 | Pa×s | 549.64 | Joback Method |
| dvisc | 0.0001196 | Pa×s | 599.99 | Joback Method |
| dvisc | 0.0000913 | Pa×s | 650.34 | Joback Method |
| dvisc | 0.0000724 | Pa×s | 700.68 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C120116&Units=SI
**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

# 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

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|---|---|
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |