

[1,1'-Biphenyl]-2,2'-diol, 3,3'-dimethoxy-5,5'-di-2-propenyl-

Other names: 2,2'-Biphenyldiol, 5,5'-diallyl-3,3'-dimethoxy-Dehydrodieugenol

5,5'-Diallyl-3,3'-dimethoxy-[1,1'-biphenyl]-2,2'-diol

Inchi: InChI=1S/C20H22O4/c1-5-7-13-9-15(19(21)17(11-13)23-3)16-10-14(8-6-2)12-18(24-4)20

InchiKey: KETPSFSOGFKJJY-UHFFFAOYSA-N

Formula: C20H22O4

SMILES: C=CCc1cc(OC)c(O)c(-c2cc(CC=C)cc(OC)c2O)c1

Mol. weight [g/mol]: 326.39

CAS: 4433-08-3

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -39.74 | kJ/mol | Joback Method |
| hf | -397.15 | kJ/mol | Joback Method |
| hfus | 45.46 | kJ/mol | Joback Method |
| hvap | 96.82 | kJ/mol | Joback Method |
| log10ws | -5.56 | | Crippen Method |
| logp | 4.239 | | Crippen Method |
| mcvol | 260.020 | ml/mol | McGowan Method |
| pc | 2088.84 | kPa | Joback Method |
| rinpol | 2707.70 | | NIST Webbook |
| rinpol | 2707.70 | | NIST Webbook |
| tb | 929.72 | K | Joback Method |
| tc | 1165.94 | K | Joback Method |
| tf | 682.46 | K | Joback Method |
| vc | 0.870 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 800.21 | J/molxK | 929.72 | Joback Method |
| cpg | 815.23 | J/molxK | 969.09 | Joback Method |
| cpg | 829.87 | J/molxK | 1008.46 | Joback Method |
| cpg | 844.28 | J/molxK | 1047.83 | Joback Method |

| | | | | |
|-------|-----------|---------|---------|---------------|
| cpg | 858.58 | J/molxK | 1087.20 | Joback Method |
| cpg | 872.92 | J/molxK | 1126.57 | Joback Method |
| cpg | 887.42 | J/molxK | 1165.94 | Joback Method |
| dvisc | 0.0000019 | Paxs | 682.46 | Joback Method |
| dvisc | 0.0000010 | Paxs | 723.67 | Joback Method |
| dvisc | 0.0000006 | Paxs | 764.88 | Joback Method |
| dvisc | 0.0000004 | Paxs | 806.09 | Joback Method |
| dvisc | 0.0000002 | Paxs | 847.30 | Joback Method |
| dvisc | 0.0000002 | Paxs | 888.51 | Joback Method |
| dvisc | 0.0000001 | Paxs | 929.72 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4433083&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| 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 |

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