

Phenol, 4-(3-hydroxy-1-propenyl)-2-methoxy-

| | |
|-----------------------------|---|
| Other names: | 2-Propen-1-ol, 3-(4-hydroxy-3-methoxyphenyl)- «gamma»-Hydroxyisoeugenol p-Hydroxy-m-methoxycinnamyl alcohol Coniferol Coniferyl alcohol 4-Hydroxy-3-methoxycinnamic alcohol 3-(4-Hydroxy-3-methoxyphenyl)-2-propen-1-ol 3-(4-Hydroxy-3-methoxyphenyl)allyl alcohol 4-[3-Hydroxy-1-propenyl]-2-methoxyphenol Coniferylic alcohol Phenol, 4-(3-hydroxy-1-propen-1-yl)-2-methoxy- 4-hydroxy-3-methoxycinnamylic alcohol |
| Inchi: | InChI=1S/C10H12O3/c1-13-10-7-8(3-2-6-11)4-5-9(10)12/h2-5,7,11-12H,6H2,1H3 |
| InchiKey: | JMFRWRFFLBVWSI-UHFFFAOYSA-N |
| Formula: | C10H12O3 |
| SMILES: | COc1cc(C=CCO)ccc1O |
| Mol. weight [g/mol]: | 180.20 |
| CAS: | 458-35-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -180.12 | kJ/mol | Joback Method |
| hf | -369.21 | kJ/mol | Joback Method |
| hfus | 26.57 | kJ/mol | Joback Method |
| hvap | 72.85 | kJ/mol | Joback Method |
| log10ws | -1.65 | | Crippen Method |
| logp | 1.406 | | Crippen Method |
| mvol | 141.310 | ml/mol | McGowan Method |
| pc | 3975.52 | kPa | Joback Method |
| rinpol | 1726.00 | | NIST Webbook |
| rinpol | 1663.00 | | NIST Webbook |
| rinpol | 1729.00 | | NIST Webbook |
| rinpol | 1688.00 | | NIST Webbook |
| rinpol | 1685.00 | | NIST Webbook |
| rinpol | 290.82 | | NIST Webbook |
| tb | 659.24 | K | Joback Method |
| tc | 869.04 | K | Joback Method |

| | | | |
|----|--------|----------------------|---------------|
| tf | 431.09 | K | Joback Method |
| vc | 0.470 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 361.86 | J/mol×K | 659.24 | Joback Method |
| cpg | 371.97 | J/mol×K | 694.21 | Joback Method |
| cpg | 381.51 | J/mol×K | 729.17 | Joback Method |
| cpg | 390.53 | J/mol×K | 764.14 | Joback Method |
| cpg | 399.09 | J/mol×K | 799.11 | Joback Method |
| cpg | 407.27 | J/mol×K | 834.08 | Joback Method |
| cpg | 415.12 | J/mol×K | 869.04 | Joback Method |
| dvisc | 0.0004866 | Paxs | 431.09 | Joback Method |
| dvisc | 0.0001709 | Paxs | 469.12 | Joback Method |
| dvisc | 0.0000702 | Paxs | 507.14 | Joback Method |
| dvisc | 0.0000327 | Paxs | 545.16 | Joback Method |
| dvisc | 0.0000168 | Paxs | 583.19 | Joback Method |
| dvisc | 0.0000094 | Paxs | 621.22 | Joback Method |
| dvisc | 0.0000056 | Paxs | 659.24 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 437.20 | K | 0.40 | NIST Webbook |

Sources

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

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C458355&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 |
| 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 |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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