

# Phenol, 2-methoxy-4-(1-propenyl)-, (Z)-

|                      |                                                                                                                                                                                                                                                                                                                                                      |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Phenol, 2-methoxy-4-propenyl-, (Z)-<br>cis-Isoeugenol<br>cis-2-Methoxy-4-propenylphenol<br>Isoeugenol, Z-<br>2-Methoxy-4-[(1Z)-1-propenyl]phenol<br>4-(1-Propenyl)-2-methoxyphenol, (Z)-<br>(Z)-Isoeugenol<br>(Z)-2-Methoxy-4-(prop-1-enyl)phenol<br>cis-4-Propenylguaiacol<br>1-(2-furanyl)-2-hydroxyethanone<br>(Z)-2-Methoxy-5-(1-propenyl)phenol |
| Inchi:               | InChI=1S/C10H12O2/c1-3-4-8-5-6-9(11)10(7-8)12-2/h3-7,11H,1-2H3/b4-3-                                                                                                                                                                                                                                                                                 |
| InchiKey:            | BJIOGJUNALELMI-ARJAWSKDSA-N                                                                                                                                                                                                                                                                                                                          |
| Formula:             | C10H12O2                                                                                                                                                                                                                                                                                                                                             |
| SMILES:              | CC=Cc1ccc(O)c(OC)c1                                                                                                                                                                                                                                                                                                                                  |
| Mol. weight [g/mol]: | 164.20                                                                                                                                                                                                                                                                                                                                               |
| CAS:                 | 5912-86-7                                                                                                                                                                                                                                                                                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -43.30  | kJ/mol | Joback Method  |
| hf            | -216.98 | kJ/mol | Joback Method  |
| hfus          | 22.48   | kJ/mol | Joback Method  |
| hvap          | 56.17   | kJ/mol | Joback Method  |
| log10ws       | -2.38   |        | Crippen Method |
| logp          | 2.434   |        | Crippen Method |
| mcvol         | 135.440 | ml/mol | McGowan Method |
| pc            | 3551.53 | kPa    | Joback Method  |
| rinpol        | 1408.00 |        | NIST Webbook   |
| rinpol        | 1423.00 |        | NIST Webbook   |
| rinpol        | 1376.00 |        | NIST Webbook   |
| rinpol        | 1402.00 |        | NIST Webbook   |
| rinpol        | 1370.00 |        | NIST Webbook   |
| rinpol        | 1407.00 |        | NIST Webbook   |
| rinpol        | 1415.00 |        | NIST Webbook   |
| rinpol        | 1366.00 |        | NIST Webbook   |
| rinpol        | 1379.00 |        | NIST Webbook   |

|        |         |         |               |
|--------|---------|---------|---------------|
| rinpol | 1392.00 |         | NIST Webbook  |
| rinpol | 1407.00 |         | NIST Webbook  |
| rinpol | 1397.00 |         | NIST Webbook  |
| rinpol | 1423.00 |         | NIST Webbook  |
| rinpol | 1402.00 |         | NIST Webbook  |
| rinpol | 1423.00 |         | NIST Webbook  |
| ripol  | 2298.00 |         | NIST Webbook  |
| ripol  | 2256.00 |         | NIST Webbook  |
| ripol  | 2270.00 |         | NIST Webbook  |
| ripol  | 2230.00 |         | NIST Webbook  |
| ripol  | 2240.00 |         | NIST Webbook  |
| ripol  | 2270.00 |         | NIST Webbook  |
| ripol  | 2226.00 |         | NIST Webbook  |
| ripol  | 2288.00 |         | NIST Webbook  |
| ripol  | 2256.00 |         | NIST Webbook  |
| ripol  | 2264.00 |         | NIST Webbook  |
| ripol  | 2281.00 |         | NIST Webbook  |
| ripol  | 2310.00 |         | NIST Webbook  |
| ripol  | 2258.00 |         | NIST Webbook  |
| ripol  | 2281.00 |         | NIST Webbook  |
| ripol  | 2287.00 |         | NIST Webbook  |
| tb     | 567.06  | K       | Joback Method |
| tc     | 793.89  | K       | Joback Method |
| tf     | 370.27  | K       | Joback Method |
| vc     | 0.452   | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 379.83    | J/mol×K | 793.89          | Joback Method |
| cpg           | 370.65    | J/mol×K | 756.09          | Joback Method |
| cpg           | 360.95    | J/mol×K | 718.28          | Joback Method |
| cpg           | 350.65    | J/mol×K | 680.48          | Joback Method |
| cpg           | 339.68    | J/mol×K | 642.67          | Joback Method |
| cpg           | 327.96    | J/mol×K | 604.87          | Joback Method |
| cpg           | 315.41    | J/mol×K | 567.06          | Joback Method |
| dvisc         | 0.0012214 | Pa×s    | 370.27          | Joback Method |
| dvisc         | 0.0000332 | Pa×s    | 567.06          | Joback Method |
| dvisc         | 0.0000504 | Pa×s    | 534.26          | Joback Method |
| dvisc         | 0.0000807 | Pa×s    | 501.46          | Joback Method |
| dvisc         | 0.0001380 | Pa×s    | 468.67          | Joback Method |

|       |           |        |        |               |
|-------|-----------|--------|--------|---------------|
| dvisc | 0.0002559 | Pa×s   | 435.87 | Joback Method |
| dvisc | 0.0005246 | Pa×s   | 403.07 | Joback Method |
| hvapt | 69.70     | kJ/mol | 388.00 | NIST Webbook  |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5912867&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5912867&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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