

# zingerol

|                      |                                                                               |
|----------------------|-------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C11H16O3/c1-8(12)3-4-9-5-6-10(13)11(7-9)14-2/h5-8,12-13H,3-4H2,1-2H3 |
| InchiKey:            | GTLGHKNKLRZSMO-UHFFFAOYSA-N                                                   |
| Formula:             | C11H16O3                                                                      |
| SMILES:              | COc1cc(CCC(C)O)ccc1O                                                          |
| Mol. weight [g/mol]: | 196.24                                                                        |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -254.36 | kJ/mol  | Joback Method  |
| hf            | -512.35 | kJ/mol  | Joback Method  |
| hfus          | 25.43   | kJ/mol  | Joback Method  |
| hvap          | 74.73   | kJ/mol  | Joback Method  |
| log10ws       | -2.15   |         | Crippen Method |
| logp          | 1.714   |         | Crippen Method |
| mcvol         | 159.700 | ml/mol  | McGowan Method |
| pc            | 3356.75 | kPa     | Joback Method  |
| ripol         | 2908.00 |         | NIST Webbook   |
| ripol         | 2908.00 |         | NIST Webbook   |
| ripol         | 2910.00 |         | NIST Webbook   |
| tb            | 677.52  | K       | Joback Method  |
| tc            | 880.57  | K       | Joback Method  |
| tf            | 432.44  | K       | Joback Method  |
| vc            | 0.540   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 434.47 | J/mol×K | 677.52          | Joback Method |
| cpg           | 446.17 | J/mol×K | 711.36          | Joback Method |
| cpg           | 457.25 | J/mol×K | 745.20          | Joback Method |
| cpg           | 467.74 | J/mol×K | 779.04          | Joback Method |
| cpg           | 477.70 | J/mol×K | 812.88          | Joback Method |
| cpg           | 487.18 | J/mol×K | 846.73          | Joback Method |
| cpg           | 496.23 | J/mol×K | 880.57          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0005700 | Pa×s | 432.44 | Joback Method |
| dvisc | 0.0001820 | Pa×s | 473.29 | Joback Method |
| dvisc | 0.0000697 | Pa×s | 514.13 | Joback Method |
| dvisc | 0.0000307 | Pa×s | 554.98 | Joback Method |
| dvisc | 0.0000152 | Pa×s | 595.83 | Joback Method |
| dvisc | 0.0000082 | Pa×s | 636.67 | Joback Method |
| dvisc | 0.0000048 | Pa×s | 677.52 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R332833&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R332833&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>                                     |

## 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>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>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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