

# Phenol, 4-[1-(1-methylpropyl)pentyl]

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C15H24O/c1-4-6-7-15(12(3)5-2)13-8-10-14(16)11-9-13/h8-12,15-16H,4-7H2,1 |
| <b>InchiKey:</b>            | WBUSLIDIERIATJ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C15H24O  |
| <b>SMILES:</b>              | CCCCC(c1ccc(O)cc1)C(C)CC   |
| <b>Mol. weight [g/mol]:</b> | 220.35   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 28.33   | kJ/mol               | Joback Method  |
| hf            | -304.27 | kJ/mol               | Joback Method  |
| hfus          | 27.38   | kJ/mol               | Joback Method  |
| hvap          | 63.50   | kJ/mol               | Joback Method  |
| log10ws       | -4.47   |                      | Crippen Method |
| logp          | 4.712   |                      | Crippen Method |
| mvol          | 204.320 | ml/mol               | McGowan Method |
| pc            | 2139.38 | kPa                  | Joback Method  |
| rinpol        | 1779.00 |                      | NIST Webbook   |
| tb            | 649.02  | K                    | Joback Method  |
| tc            | 858.39  | K                    | Joback Method  |
| tf            | 366.95  | K                    | Joback Method  |
| vc            | 0.722   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 558.51    | J/molxK | 649.02          | Joback Method |
| cpg           | 636.64    | J/molxK | 823.49          | Joback Method |
| cpg           | 622.73    | J/molxK | 788.60          | Joback Method |
| cpg           | 608.04    | J/molxK | 753.70          | Joback Method |
| cpg           | 592.50    | J/molxK | 718.81          | Joback Method |
| cpg           | 576.02    | J/molxK | 683.91          | Joback Method |
| cpg           | 649.87    | J/molxK | 858.39          | Joback Method |
| dvisc         | 0.0000169 | Paxs    | 649.02          | Joback Method |
| dvisc         | 0.0000285 | Paxs    | 602.01          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000525 | Paxs | 555.00 | Joback Method |
| dvisc | 0.0001083 | Paxs | 507.99 | Joback Method |
| dvisc | 0.0002590 | Paxs | 460.97 | Joback Method |
| dvisc | 0.0007553 | Paxs | 413.96 | Joback Method |
| dvisc | 0.0028979 | Paxs | 366.95 | 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=R592426&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R592426&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>rinpol:</b>  | Non-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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