

# Phenol, 4-[1,3-dimethyl-2-(1-methylethyl)butyl]

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24O/c1-10(2)15(11(3)4)12(5)13-6-8-14(16)9-7-13/h6-12,15-16H,1-5H3

KMYWIMJCAIAOPT-UHFFFAOYSA-N

C15H24O

CC(C)C(C(C)C)C(C)c1ccc(O)cc1

220.35

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 23.45   | kJ/mol  | Joback Method  |
| hf            | -314.83 | kJ/mol  | Joback Method  |
| hfus          | 20.34   | kJ/mol  | Joback Method  |
| hvap          | 62.72   | kJ/mol  | Joback Method  |
| log10ws       | -3.99   |         | Crippen Method |
| logp          | 4.424   |         | Crippen Method |
| mcvol         | 204.320 | ml/mol  | McGowan Method |
| pc            | 2171.40 | kPa     | Joback Method  |
| rinpol        | 1746.00 |         | NIST Webbook   |
| tb            | 648.14  | K       | Joback Method  |
| tc            | 865.70  | K       | Joback Method  |
| tf            | 336.95  | K       | Joback Method  |
| vc            | 0.710   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 559.41    | J/mol×K | 648.14          | Joback Method |
| cpg           | 640.43    | J/mol×K | 829.44          | Joback Method |
| cpg           | 626.10    | J/mol×K | 793.18          | Joback Method |
| cpg           | 610.93    | J/mol×K | 756.92          | Joback Method |
| cpg           | 594.82    | J/mol×K | 720.66          | Joback Method |
| cpg           | 577.68    | J/mol×K | 684.40          | Joback Method |
| cpg           | 654.00    | J/mol×K | 865.70          | Joback Method |
| dvisc         | 0.0000146 | Pa×s    | 648.14          | Joback Method |
| dvisc         | 0.0000265 | Pa×s    | 596.27          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000537 | Pa×s | 544.41 | Joback Method |
| dvisc | 0.0001262 | Pa×s | 492.54 | Joback Method |
| dvisc | 0.0003630 | Pa×s | 440.68 | Joback Method |
| dvisc | 0.0013836 | Pa×s | 388.81 | Joback Method |
| dvisc | 0.0079615 | Pa×s | 336.95 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R592595&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R592595&amp;Units=SI</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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