

# Phenol, 4-[3-methyl-1-(2-methylpropyl)butyl]

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24O/c1-11(2)9-14(10-12(3)4)13-5-7-15(16)8-6-13/h5-8,11-12,14,16H,9-1

XCXFTADVDUIGMI-UHFFFAOYSA-N

C15H24O

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

220.35

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 25.89   | kJ/mol  | Joback Method  |
| hf            | -309.55 | kJ/mol  | Joback Method  |
| hfus          | 23.86   | kJ/mol  | Joback Method  |
| hvap          | 63.11   | kJ/mol  | Joback Method  |
| log10ws       | -4.23   |         | Crippen Method |
| logp          | 4.568   |         | Crippen Method |
| mcvol         | 204.320 | ml/mol  | McGowan Method |
| pc            | 2155.30 | kPa     | Joback Method  |
| rinpol        | 1695.00 |         | NIST Webbook   |
| rinpol        | 1695.00 |         | NIST Webbook   |
| tb            | 648.58  | K       | Joback Method  |
| tc            | 861.97  | K       | Joback Method  |
| tf            | 351.95  | K       | Joback Method  |
| vc            | 0.716   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 558.96    | J/mol×K | 648.58          | Joback Method |
| cpg           | 576.84    | J/mol×K | 684.14          | Joback Method |
| cpg           | 593.65    | J/mol×K | 719.71          | Joback Method |
| cpg           | 609.47    | J/mol×K | 755.27          | Joback Method |
| cpg           | 624.40    | J/mol×K | 790.84          | Joback Method |
| cpg           | 638.52    | J/mol×K | 826.40          | Joback Method |
| cpg           | 651.91    | J/mol×K | 861.97          | Joback Method |
| dvisc         | 0.0046742 | Pa×s    | 351.95          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0010084 | Pa×s | 401.39 | Joback Method |
| dvisc | 0.0003045 | Pa×s | 450.83 | Joback Method |
| dvisc | 0.0001165 | Pa×s | 500.26 | Joback Method |
| dvisc | 0.0000530 | Pa×s | 549.70 | Joback Method |
| dvisc | 0.0000275 | Pa×s | 599.14 | Joback Method |
| dvisc | 0.0000157 | Pa×s | 648.58 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=R593201&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R593201&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>                                 |

## 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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