

# Phenol, 4,4'-(1-methylethylidene)bis[2-methyl-

|                      |                                                                                                                                                                                                                                                                                                                                                                                               |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2,2-Bis(3-methyl-4-hydroxyphenyl)propane<br>Phenol, 4,4'-(1-methylethylidene)bis[2-methyl-<br>o-Cresol, 4,4'-isopropylidenedi-<br>Dicresylolpropane<br>Nonox DCP<br>2,2-Bis(4-hydroxy-3-methylphenyl)propane<br>3,3'-Dimethyldian<br>4,4'-Isopropylidenebis[2-methylphenol]<br>4,4'-Isopropylidenedi-o-cresol<br>o-Cresol, 4,4'-(2,2-propylene)bis-<br>3,3'-Dimethylbisphenol A<br>NSC 408489 |
| Inchi:               | InChI=1S/C17H20O2/c1-11-9-13(5-7-15(11)18)17(3,4)14-6-8-16(19)12(2)10-14/h5-10,18                                                                                                                                                                                                                                                                                                             |
| InchiKey:            | YMTYZTXUZLQUSF-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                                                   |
| Formula:             | C17H20O2                                                                                                                                                                                                                                                                                                                                                                                      |
| SMILES:              | Cc1cc(C(C)(C)c2ccc(O)c(C)c2)ccc1O                                                                                                                                                                                                                                                                                                                                                             |
| Mol. weight [g/mol]: | 256.35                                                                                                                                                                                                                                                                                                                                                                                        |

## Physical Properties

| Property code | Value   | Unit    | Source             |
|---------------|---------|---------|--------------------|
| af            | 0.7462  |         | Cheméo Relay (1.0) |
| gf            | -8.58   | kJ/mol  | Joback Method      |
| hf            | -272.69 | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 31.24   | kJ/mol  | Joback Method      |
| hvap          | 120.65  | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 7.67    | eV      | Cheméo Relay (1.0) |
| log10ws       | -4.02   |         | Cheméo Relay (1.0) |
| logp          | 4.041   |         | Crippen Method     |
| mcvol         | 214.610 | ml/mol  | McGowan Method     |
| pc            | 2767.17 | kPa     | Joback Method      |
| tb            | 581.95  | K       | Cheméo Relay (1.0) |
| tc            | 911.02  | K       | Cheméo Relay (1.0) |
| tf            | 407.63  | K       | Cheméo Relay (1.0) |
| vc            | 0.752   | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 633.88    | J/mol×K | 809.69          | Joback Method |
| cpg           | 649.15    | J/mol×K | 852.09          | Joback Method |
| cpg           | 663.85    | J/mol×K | 894.49          | Joback Method |
| cpg           | 678.23    | J/mol×K | 936.89          | Joback Method |
| cpg           | 692.53    | J/mol×K | 979.29          | Joback Method |
| cpg           | 706.98    | J/mol×K | 1021.69         | Joback Method |
| cpg           | 721.84    | J/mol×K | 1064.09         | Joback Method |
| dvisc         | 0.0000113 | Pa×s    | 585.09          | Joback Method |
| dvisc         | 0.0000054 | Pa×s    | 622.52          | Joback Method |
| dvisc         | 0.0000028 | Pa×s    | 659.96          | Joback Method |
| dvisc         | 0.0000016 | Pa×s    | 697.39          | Joback Method |
| dvisc         | 0.0000009 | Pa×s    | 734.82          | Joback Method |
| dvisc         | 0.0000006 | Pa×s    | 772.26          | Joback Method |
| dvisc         | 0.0000004 | Pa×s    | 809.69          | Joback Method |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 514.20 | K    | 1.60           | NIST Webbook |

## Sources

|                           |                                                                                                                                         |
|---------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                   |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                   |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                               |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                       |
| Cheméo Relay (1.0):       |                                                                                                                                         |
| Cheméo Relay (1.0, beta): |                                                                                                                                         |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C79970&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C79970&amp;Units=SI</a> |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>af:</b>      | Acentric Factor                                 |
| <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>ie:</b>      | Ionization energy                               |
| <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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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