

# «alpha»,«alpha»,«alpha»',«alpha»'-Tetramethyl-1,

|                      |                                                                                                                                                                                                                                                                     |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | «alpha»,«alpha»'-Dihydroxy-p-diisopropylbenzene<br>1,4-Benzenedimethanol, «alpha»,«alpha»,«alpha»',«alpha»'-tetramethyl-alpha,alpha,alpha',alpha'-Tetramethyl-1,4-benzenedimethanol<br>«alpha»,«alpha»,«alpha»',«alpha»'-tetramethyl-p-xylene-«alpha»,«alpha»'-diol |
| Inchi:               | InChI=1S/C12H18O2/c1-11(2,13)9-5-7-10(8-6-9)12(3,4)14/h5-8,13-14H,1-4H3                                                                                                                                                                                             |
| InchiKey:            | LEARFTRDZQQTDN-UHFFFAOYSA-N                                                                                                                                                                                                                                         |
| Formula:             | C12H18O2                                                                                                                                                                                                                                                            |
| SMILES:              | CC(C)(O)c1ccc(C(C)(C)O)cc1                                                                                                                                                                                                                                          |
| Mol. weight [g/mol]: | 194.27                                                                                                                                                                                                                                                              |
| CAS:                 | 2948-46-1                                                                                                                                                                                                                                                           |

## Physical Properties

| Property code | Value           | Unit    | Source         |
|---------------|-----------------|---------|----------------|
| chs           | -6751.60 ± 1.40 | kJ/mol  | NIST Webbook   |
| gf            | -115.02         | kJ/mol  | Joback Method  |
| hf            | -387.91         | kJ/mol  | Joback Method  |
| hfs           | -543.00 ± 1.50  | kJ/mol  | NIST Webbook   |
| hfus          | 13.84           | kJ/mol  | Joback Method  |
| hsub          | 136.80 ± 2.80   | kJ/mol  | NIST Webbook   |
| hvap          | 76.01           | kJ/mol  | Joback Method  |
| log10ws       | -2.78           |         | Crippen Method |
| logp          | 2.141           |         | Crippen Method |
| mcvol         | 167.920         | ml/mol  | McGowan Method |
| pc            | 2979.54         | kPa     | Joback Method  |
| tb            | 683.52          | K       | Joback Method  |
| tc            | 881.33          | K       | Joback Method  |
| tf            | 390.42          | K       | Joback Method  |
| vc            | 0.616           | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 468.07 | J/mol×K | 683.52          | Joback Method |
| cpg           | 480.04 | J/mol×K | 716.49          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 491.22    | J/mol×K | 749.46 | Joback Method |
| cpg   | 501.68    | J/mol×K | 782.42 | Joback Method |
| cpg   | 511.48    | J/mol×K | 815.39 | Joback Method |
| cpg   | 520.68    | J/mol×K | 848.36 | Joback Method |
| cpg   | 529.35    | J/mol×K | 881.33 | Joback Method |
| dvisc | 0.0036683 | Pa×s    | 390.42 | Joback Method |
| dvisc | 0.0008008 | Pa×s    | 439.27 | Joback Method |
| dvisc | 0.0002371 | Pa×s    | 488.12 | Joback Method |
| dvisc | 0.0000876 | Pa×s    | 536.97 | Joback Method |
| dvisc | 0.0000382 | Pa×s    | 585.82 | Joback Method |
| dvisc | 0.0000189 | Pa×s    | 634.67 | Joback Method |
| dvisc | 0.0000104 | Pa×s    | 683.52 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2948461&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2948461&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>                                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|                 |                                                          |
|-----------------|----------------------------------------------------------|
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <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>hfs:</b>     | Solid phase enthalpy of formation at standard conditions |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions                |
| <b>hsub:</b>    | Enthalpy of sublimation 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>tb:</b>      | Normal Boiling Point Temperature                         |
| <b>tc:</b>      | Critical Temperature                                     |

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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