

Phenol, 4-(1,1,2,3-tetramethylpentyl), diastereomer # 1

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|----------------------|---|
| Inchi: | InChI=1S/C15H24O/c1-6-11(2)12(3)15(4,5)13-7-9-14(16)10-8-13/h7-12,16H,6H2,1-5H3 |
| InchiKey: | HGQNCRWGYCBKAU-UHFFFAOYSA-N |
| Formula: | C15H24O |
| SMILES: | CCC(C)C(C)C(C)(C)c1ccc(O)cc1 |
| Mol. weight [g/mol]: | 220.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 31.17 | kJ/mol | Joback Method |
| hf | -313.02 | kJ/mol | Joback Method |
| hfus | 19.97 | kJ/mol | Joback Method |
| hvap | 62.20 | kJ/mol | Joback Method |
| log10ws | -3.94 | | Crippen Method |
| logp | 4.352 | | Crippen Method |
| mcvol | 204.320 | ml/mol | McGowan Method |
| pc | 2177.49 | kPa | Joback Method |
| rinpol | 1733.00 | | NIST Webbook |
| rinpol | 1733.00 | | NIST Webbook |
| tb | 645.79 | K | Joback Method |
| tc | 866.98 | K | Joback Method |
| tf | 369.37 | K | Joback Method |
| vc | 0.711 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 561.35 | J/molxK | 645.79 | Joback Method |
| cpg | 641.94 | J/molxK | 830.11 | Joback Method |
| cpg | 627.76 | J/molxK | 793.25 | Joback Method |
| cpg | 612.74 | J/molxK | 756.38 | Joback Method |
| cpg | 596.74 | J/molxK | 719.52 | Joback Method |
| cpg | 579.65 | J/molxK | 682.65 | Joback Method |
| cpg | 655.38 | J/molxK | 866.98 | Joback Method |
| dvisc | 0.0000148 | Paxs | 645.79 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000256 | Paxs | 599.72 | Joback Method |
| dvisc | 0.0000484 | Paxs | 553.65 | Joback Method |
| dvisc | 0.0001026 | Paxs | 507.58 | Joback Method |
| dvisc | 0.0002529 | Paxs | 461.51 | Joback Method |
| dvisc | 0.0007611 | Paxs | 415.44 | Joback Method |
| dvisc | 0.0030151 | Paxs | 369.37 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R592035&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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