

Phenol, 4-(1,5,5-trimethylhexyl)

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

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 33.61 | kJ/mol | Joback Method |
| hf | -307.74 | kJ/mol | Joback Method |
| hfus | 23.49 | kJ/mol | Joback Method |
| hvap | 62.59 | kJ/mol | Joback Method |
| log10ws | -4.47 | | Crippen Method |
| logp | 4.712 | | Crippen Method |
| mcvol | 204.320 | ml/mol | McGowan Method |
| pc | 2161.32 | kPa | Joback Method |
| rinpol | 1698.00 | | NIST Webbook |
| rinpol | 1698.00 | | NIST Webbook |
| rinpol | 1698.00 | | NIST Webbook |
| tb | 646.23 | K | Joback Method |
| tc | 863.09 | K | Joback Method |
| tf | 384.37 | K | Joback Method |
| vc | 0.717 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 560.90 | J/molxK | 646.23 | Joback Method |
| cpg | 578.81 | J/molxK | 682.37 | Joback Method |
| cpg | 595.55 | J/molxK | 718.52 | Joback Method |
| cpg | 611.26 | J/molxK | 754.66 | Joback Method |
| cpg | 626.04 | J/molxK | 790.81 | Joback Method |
| cpg | 640.01 | J/molxK | 826.95 | Joback Method |
| cpg | 653.27 | J/molxK | 863.09 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0019247 | Paxs | 384.37 | Joback Method |
| dvisc | 0.0005760 | Paxs | 428.01 | Joback Method |
| dvisc | 0.0002155 | Paxs | 471.66 | Joback Method |
| dvisc | 0.0000953 | Paxs | 515.30 | Joback Method |
| dvisc | 0.0000478 | Paxs | 558.94 | Joback Method |
| dvisc | 0.0000265 | Paxs | 602.59 | Joback Method |
| dvisc | 0.0000159 | Paxs | 646.23 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R592253&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| mcvol: | 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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