

Phenol, 4-(2-ethyl-1-methylhexyl)

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|-----------------------------|--|
| Inchi: | InChI=1S/C15H24O/c1-4-6-7-13(5-2)12(3)14-8-10-15(16)11-9-14/h8-13,16H,4-7H2,1-3H |
| InchiKey: | GSSYEGRAMDNVJA-UHFFFAOYSA-N |
| Formula: | C15H24O |
| SMILES: | CCCCC(CC)C(C)c1ccc(O)cc1 |
| Mol. weight [g/mol]: | 220.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 28.33 | kJ/mol | Joback Method |
| hf | -304.27 | kJ/mol | Joback Method |
| hfus | 27.38 | kJ/mol | Joback Method |
| hvap | 63.50 | kJ/mol | Joback Method |
| log10ws | -4.47 | | Crippen Method |
| logp | 4.712 | | Crippen Method |
| mcvol | 204.320 | ml/mol | McGowan Method |
| pc | 2139.38 | kPa | Joback Method |
| rinsol | 1766.00 | | NIST Webbook |
| tb | 649.02 | K | Joback Method |
| tc | 858.39 | K | Joback Method |
| tf | 366.95 | K | Joback Method |
| vc | 0.722 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 558.51 | J/molxK | 649.02 | Joback Method |
| cpg | 636.64 | J/molxK | 823.49 | Joback Method |
| cpg | 622.73 | J/molxK | 788.60 | Joback Method |
| cpg | 608.04 | J/molxK | 753.70 | Joback Method |
| cpg | 592.50 | J/molxK | 718.81 | Joback Method |
| cpg | 576.02 | J/molxK | 683.91 | Joback Method |
| cpg | 649.87 | J/molxK | 858.39 | Joback Method |
| dvisc | 0.0000169 | Paxs | 649.02 | Joback Method |
| dvisc | 0.0000285 | Paxs | 602.01 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000525 | Paxs | 555.00 | Joback Method |
| dvisc | 0.0001083 | Paxs | 507.99 | Joback Method |
| dvisc | 0.0002590 | Paxs | 460.97 | Joback Method |
| dvisc | 0.0007553 | Paxs | 413.96 | Joback Method |
| dvisc | 0.0028979 | Paxs | 366.95 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R593058&Units=SI |

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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<https://www.chemeo.com/cid/60-118-4/Phenol-4-2-ethyl-1-methylhexyl.pdf>

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