

Phenol, 2-(1-phenylethyl)-

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|-----------------------------|---|
| Other names: | o-(«alpha»-Methylbenzyl)phenol o-(1-Phenylethyl)phenol Phenol, o-(«alpha»-methylbenzyl)- 1-(2-Hydroxyphenyl)-1-phenylethane 2-(«alpha»-Methylbenzyl)phenol 2-(1-Phenylethyl)phenol |
| Inchi: | InChI=1S/C14H14O/c1-11(12-7-3-2-4-8-12)13-9-5-6-10-14(13)15/h2-11,15H,1H3 |
| InchiKey: | WYZIVNCBUWDCOZ-UHFFFAOYSA-N |
| Formula: | C14H14O |
| SMILES: | CC(c1ccccc1)c1ccccc1O |
| Mol. weight [g/mol]: | 198.26 |
| CAS: | 4237-44-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 134.76 | kJ/mol | Joback Method |
| hf | -41.82 | kJ/mol | Joback Method |
| hfus | 22.36 | kJ/mol | Joback Method |
| hvap | 63.94 | kJ/mol | Joback Method |
| log10ws | -3.50 | | Crippen Method |
| logp | 3.544 | | Crippen Method |
| mcvol | 166.470 | ml/mol | McGowan Method |
| pc | 3291.59 | kPa | Joback Method |
| rinpol | 1721.00 | | NIST Webbook |
| rinpol | 1683.60 | | NIST Webbook |
| rinpol | 1721.00 | | NIST Webbook |
| rinpol | 1683.60 | | NIST Webbook |
| tb | 653.26 | K | Joback Method |
| tc | 907.43 | K | Joback Method |
| tf | 397.10 | K | Joback Method |
| vc | 0.564 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 427.10 | J/mol×K | 653.26 | Joback Method |
| cpg | 494.33 | J/mol×K | 865.07 | Joback Method |
| cpg | 482.79 | J/mol×K | 822.71 | Joback Method |
| cpg | 470.46 | J/mol×K | 780.35 | Joback Method |
| cpg | 457.16 | J/mol×K | 737.98 | Joback Method |
| cpg | 442.76 | J/mol×K | 695.62 | Joback Method |
| cpg | 505.21 | J/mol×K | 907.43 | Joback Method |
| dvisc | 0.0000196 | Paxs | 653.26 | Joback Method |
| dvisc | 0.0000309 | Paxs | 610.57 | Joback Method |
| dvisc | 0.0000521 | Paxs | 567.87 | Joback Method |
| dvisc | 0.0000956 | Paxs | 525.18 | Joback Method |
| dvisc | 0.0001955 | Paxs | 482.49 | Joback Method |
| dvisc | 0.0004594 | Paxs | 439.79 | Joback Method |
| dvisc | 0.0012972 | Paxs | 397.10 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4237449&Units=SI |
| 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 |

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 |
| rinpola: | 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/78-509-1/Phenol-2-1-phenylethyl.pdf>

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