

3-Butene-2-one-4-ol, 1,4-diphenyl-

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|-----------------------------|---|
| Inchi: | InChI=1S/C16H14O2/c17-15(11-13-7-3-1-4-8-13)12-16(18)14-9-5-2-6-10-14/h1-10,12,18 |
| InchiKey: | GUHCMRKVXZWKCO-VBKFSLOCSA-N |
| Formula: | C16H14O2 |
| SMILES: | O=C(C=C(O)c1ccccc1)Cc1ccccc1 |
| Mol. weight [g/mol]: | 238.28 |
| CAS: | 3442-15-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 114.59 | kJ/mol | Joback Method |
| hf | -57.89 | kJ/mol | Joback Method |
| hfus | 29.86 | kJ/mol | Joback Method |
| hvap | 79.23 | kJ/mol | Joback Method |
| ie | 8.36 | eV | NIST Webbook |
| log10ws | -3.85 | | Crippen Method |
| logp | 3.397 | | Crippen Method |
| mcvol | 191.920 | ml/mol | McGowan Method |
| pc | 2829.33 | kPa | Joback Method |
| tb | 768.93 | K | Joback Method |
| tc | 998.58 | K | Joback Method |
| tf | 414.63 | K | Joback Method |
| vc | 0.722 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 521.68 | J/molxK | 768.93 | Joback Method |
| cpg | 534.20 | J/molxK | 807.21 | Joback Method |
| cpg | 545.76 | J/molxK | 845.48 | Joback Method |
| cpg | 556.45 | J/molxK | 883.76 | Joback Method |
| cpg | 566.37 | J/molxK | 922.03 | Joback Method |
| cpg | 575.61 | J/molxK | 960.31 | Joback Method |
| cpg | 584.26 | J/molxK | 998.58 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C3442157&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| cpg: | Ideal gas heat capacity |
| 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 |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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