

2,3-diphenyl-1-butene

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|-----------------------------|---|
| Inchi: | InChI=1S/C16H16/c1-13(15-9-5-3-6-10-15)14(2)16-11-7-4-8-12-16/h3-12,14H,1H2,2H3 |
| InchiKey: | YDLBGKXKYRMYHL-UHFFFAOYSA-N |
| Formula: | C16H16 |
| SMILES: | <chem>C=C(c1ccccc1)C(C)c1ccccc1</chem> |
| Mol. weight [g/mol]: | 208.30 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 385.51 | kJ/mol | Joback Method |
| hf | 209.85 | kJ/mol | Joback Method |
| hfus | 19.17 | kJ/mol | Joback Method |
| hvap | 54.78 | kJ/mol | Joback Method |
| log10ws | -4.71 | | Crippen Method |
| logp | 4.503 | | Crippen Method |
| mcvol | 184.480 | ml/mol | McGowan Method |
| pc | 2410.00 | kPa | Joback Method |
| rinpol | 1610.40 | | NIST Webbook |
| rinpol | 1610.40 | | NIST Webbook |
| tb | 614.96 | K | Joback Method |
| tc | 859.57 | K | Joback Method |
| tf | 292.20 | K | Joback Method |
| vc | 0.692 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 450.87 | J/mol×K | 614.96 | Joback Method |
| cpg | 469.71 | J/mol×K | 655.73 | Joback Method |
| cpg | 487.07 | J/mol×K | 696.50 | Joback Method |
| cpg | 503.03 | J/mol×K | 737.26 | Joback Method |
| cpg | 517.71 | J/mol×K | 778.03 | Joback Method |
| cpg | 531.21 | J/mol×K | 818.80 | Joback Method |
| cpg | 543.62 | J/mol×K | 859.57 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R316277&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

| | |
|-----------------|---|
| 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 |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | 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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