

Benzophenone, 2,4,6-trimethyl-

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|-----------------------------|---|
| Other names: | Ketone, mesityl phenyl Mesityl phenyl ketone Mesitylene, 2-benzoyl- Methanone, phenyl(2,4,6-trimethylphenyl)- 2,4,6-Trimethylbenzophenone 2,4,6-Trimetilbenzofenon |
| Inchi: | InChI=1S/C16H16O/c1-11-9-12(2)15(13(3)10-11)16(17)14-7-5-4-6-8-14/h4-10H,1-3H3 |
| InchiKey: | HPAFOABSQZMTHE-UHFFFAOYSA-N |
| Formula: | C16H16O |
| SMILES: | <chem>Cc1cc(C)c(C(=O)c2ccccc2)c(C)c1</chem> |
| Mol. weight [g/mol]: | 224.30 |
| CAS: | 954-16-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 150.85 | kJ/mol | Joback Method |
| hf | -47.50 | kJ/mol | Joback Method |
| hfus | 25.71 | kJ/mol | Joback Method |
| hvap | 64.49 | kJ/mol | Joback Method |
| ie | 8.00 | eV | NIST Webbook |
| ie | 8.32 | eV | NIST Webbook |
| log10ws | -4.86 | | Crippen Method |
| logp | 3.843 | | Crippen Method |
| mcvol | 190.350 | ml/mol | McGowan Method |
| pc | 2324.78 | kPa | Joback Method |
| tb | 687.65 | K | Joback Method |
| tc | 926.61 | K | Joback Method |
| tf | 410.41 | K | Joback Method |
| vc | 0.722 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 489.90 | J/molxK | 687.65 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 506.00 | J/mol×K | 727.48 | Joback Method |
| cpg | 520.93 | J/mol×K | 767.30 | Joback Method |
| cpg | 534.74 | J/mol×K | 807.13 | Joback Method |
| cpg | 547.50 | J/mol×K | 846.96 | Joback Method |
| cpg | 559.24 | J/mol×K | 886.78 | Joback Method |
| cpg | 570.04 | J/mol×K | 926.61 | Joback Method |
| dvisc | 0.0010758 | Paxs | 410.41 | Joback Method |
| dvisc | 0.0006609 | Paxs | 456.62 | Joback Method |
| dvisc | 0.0004440 | Paxs | 502.82 | Joback Method |
| dvisc | 0.0003190 | Paxs | 549.03 | Joback Method |
| dvisc | 0.0002412 | Paxs | 595.24 | Joback Method |
| dvisc | 0.0001899 | Paxs | 641.44 | Joback Method |
| dvisc | 0.0001544 | Paxs | 687.65 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C954165&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 |
| ie: | Ionization energy |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | 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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