

4,4'-Dimethoxybenzophenone

Other names:

p,p'-Dimethoxybenzophenone
Methanone, bis(4-methoxyphenyl)-
Benzophenone, 4,4'-dimethoxy-
Bis(p-methoxy)benzophenone
Bis(4-anisyl) ketone
Bis(4-methoxyphenyl)methanone
Bis(p-anisyl) ketone
Bis(p-methoxyphenyl) ketone
Di(4-methoxyphenyl) ketone
Di-p-anisyl ketone
DMBP
Bis(4-methoxyphenyl) ketone

Inchi:

InChI=1S/C15H14O3/c1-17-13-7-3-11(4-8-13)15(16)12-5-9-14(18-2)10-6-12/h3-10H,1-2H

InchiKey:

RFVHVYKVRGKLNK-UHFFFAOYSA-N

Formula:

C15H14O3

SMILES:

COc1ccc(C(=O)c2ccc(OC)cc2)cc1

Mol. weight [g/mol]:

242.27

CAS:

90-96-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -57.94 | kJ/mol | Joback Method |
| hf | -279.83 | kJ/mol | Joback Method |
| hfus | 25.89 | kJ/mol | Joback Method |
| hvap | 66.43 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 2.935 | | Crippen Method |
| mcvol | 188.000 | ml/mol | McGowan Method |
| pc | 2507.52 | kPa | Joback Method |
| tb | 704.63 | K | Joback Method |
| tc | 940.44 | K | Joback Method |
| tf | 431.08 | K | Joback Method |
| vc | 0.702 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 490.58 | J/molxK | 704.63 | Joback Method |
| cpg | 554.26 | J/molxK | 901.14 | Joback Method |
| cpg | 543.73 | J/molxK | 861.83 | Joback Method |
| cpg | 532.11 | J/molxK | 822.53 | Joback Method |
| cpg | 519.39 | J/molxK | 783.23 | Joback Method |
| cpg | 505.56 | J/molxK | 743.93 | Joback Method |
| cpg | 563.72 | J/molxK | 940.44 | Joback Method |
| dvisc | 0.0001063 | Paxs | 704.63 | Joback Method |
| dvisc | 0.0001316 | Paxs | 659.04 | Joback Method |
| dvisc | 0.0001682 | Paxs | 613.45 | Joback Method |
| dvisc | 0.0002237 | Paxs | 567.86 | Joback Method |
| dvisc | 0.0003126 | Paxs | 522.26 | Joback Method |
| dvisc | 0.0004658 | Paxs | 476.67 | Joback Method |
| dvisc | 0.0007551 | Paxs | 431.08 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C90960&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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