

Benzoin methyl ether

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| Other names: | Ethanone, 2-methoxy-1,2-diphenyl- Acetophenone, 2-methoxy-2-phenyl- Benzoin methyl ester Methyl benzoin 2-Methoxy-2-phenylacetophenone O-Methylbenzoin «alpha»-Methoxybenzyl phenyl ketone 2-Methoxy-1,2-diphenylethanone «alpha»-Methoxydeoxybenzoin Nisso Cure MBO NSC 76550 QCU 3 2-Methoxy-1,2-diphenyl-1-ethanone |
| Inchi: | InChI=1S/C15H14O2/c1-17-15(13-10-6-3-7-11-13)14(16)12-8-4-2-5-9-12/h2-11,15H,1H3 |
| InchiKey: | BQZJOQXSCSZQPS-UHFFFAOYSA-N |
| Formula: | C15H14O2 |
| SMILES: | <chem>COC(C(=O)c1ccccc1)c1ccccc1</chem> |
| Mol. weight [g/mol]: | 226.27 |
| CAS: | 3524-62-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 63.88 | kJ/mol | Joback Method |
| hf | -129.95 | kJ/mol | Joback Method |
| hfus | 21.95 | kJ/mol | Joback Method |
| hvap | 62.30 | kJ/mol | Joback Method |
| log10ws | -3.71 | | Crippen Method |
| logp | 3.257 | | Crippen Method |
| mcvol | 182.130 | ml/mol | McGowan Method |
| pc | 2651.56 | kPa | Joback Method |
| tb | 671.81 | K | Joback Method |
| tc | 914.44 | K | Joback Method |
| tf | 368.81 | K | Joback Method |
| vc | 0.677 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 467.27 | J/molxK | 671.81 | Joback Method |
| cpg | 535.55 | J/molxK | 874.00 | Joback Method |
| cpg | 524.26 | J/molxK | 833.56 | Joback Method |
| cpg | 511.85 | J/molxK | 793.13 | Joback Method |
| cpg | 498.25 | J/molxK | 752.69 | Joback Method |
| cpg | 483.41 | J/molxK | 712.25 | Joback Method |
| cpg | 545.78 | J/molxK | 914.44 | Joback Method |
| dvisc | 0.0001264 | Paxs | 671.81 | Joback Method |
| dvisc | 0.0001649 | Paxs | 621.31 | Joback Method |
| dvisc | 0.0002254 | Paxs | 570.81 | Joback Method |
| dvisc | 0.0003275 | Paxs | 520.31 | Joback Method |
| dvisc | 0.0005154 | Paxs | 469.81 | Joback Method |
| dvisc | 0.0009050 | Paxs | 419.31 | Joback Method |
| dvisc | 0.0018537 | Paxs | 368.81 | Joback Method |

Sources

| | |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3524627&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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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