

Methanone, [4-(1-methylethyl)phenyl]phenyl-

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| Other names: | Benzophenone, 4-isopropyl- p-Isopropylbenzophenone 4-Isopropylbenzophenone |
| Inchi: | InChI=1S/C16H16O/c1-12(2)13-8-10-15(11-9-13)16(17)14-6-4-3-5-7-14/h3-12H,1-2H3 |
| InchiKey: | CKFPWZPBRHQASN-UHFFFAOYSA-N |
| Formula: | C16H16O |
| SMILES: | CC(C)c1ccc(C(=O)c2ccccc2)cc1 |
| Mol. weight [g/mol]: | 224.30 |
| CAS: | 18864-76-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|----------------------|----------------|
| chl | -8464.00 ± 2.00 | kJ/mol | NIST Webbook |
| gf | 167.67 | kJ/mol | Joback Method |
| hf | -29.84 | kJ/mol | Joback Method |
| hfl | -119.00 | kJ/mol | NIST Webbook |
| hfus | 22.96 | kJ/mol | Joback Method |
| hvap | 62.78 | kJ/mol | Joback Method |
| log10ws | -4.61 | | Crippen Method |
| logp | 4.041 | | Crippen Method |
| mcvol | 190.350 | ml/mol | McGowan Method |
| pc | 2412.37 | kPa | Joback Method |
| tb | 677.25 | K | Joback Method |
| tc | 919.42 | K | Joback Method |
| tf | 370.37 | K | Joback Method |
| vc | 0.716 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 492.14 | J/mol×K | 677.25 | Joback Method |
| cpg | 563.94 | J/mol×K | 879.06 | Joback Method |
| cpg | 551.91 | J/mol×K | 838.70 | Joback Method |
| cpg | 538.79 | J/mol×K | 798.34 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 524.51 | J/mol×K | 757.97 | Joback Method |
| cpg | 508.98 | J/mol×K | 717.61 | Joback Method |
| cpg | 574.96 | J/mol×K | 919.42 | Joback Method |
| dvisc | 0.0001439 | Paxs | 677.25 | Joback Method |
| dvisc | 0.0001857 | Paxs | 626.10 | Joback Method |
| dvisc | 0.0002508 | Paxs | 574.96 | Joback Method |
| dvisc | 0.0003593 | Paxs | 523.81 | Joback Method |
| dvisc | 0.0005564 | Paxs | 472.66 | Joback Method |
| dvisc | 0.0009580 | Paxs | 421.52 | Joback Method |
| dvisc | 0.0019166 | Paxs | 370.37 | 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=C18864761&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|---|
| chl: | Standard liquid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfl: | Liquid phase 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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