

«beta»-Ethoxychalcone

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|-----------------------------|---|
| Inchi: | InChI=1S/C17H16O2/c1-2-19-17(15-11-7-4-8-12-15)13-16(18)14-9-5-3-6-10-14/h3-13H,2 |
| InchiKey: | GMWQGXUAHMDHHZ-LGMDPLHJSA-N |
| Formula: | C17H16O2 |
| SMILES: | CCOC(=CC(=O)c1cccc1)c1cccc1 |
| Mol. weight [g/mol]: | 252.31 |
| CAS: | 1907-69-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|----------------------|----------------|
| chs | -8786.00 ± 2.00 | kJ/mol | NIST Webbook |
| gf | 154.83 | kJ/mol | Joback Method |
| hf | -58.52 | kJ/mol | Joback Method |
| hfus | 29.55 | kJ/mol | Joback Method |
| hvap | 67.18 | kJ/mol | Joback Method |
| log10ws | -4.61 | | Crippen Method |
| logp | 3.947 | | Crippen Method |
| mcvol | 206.010 | ml/mol | McGowan Method |
| pc | 2300.32 | kPa | Joback Method |
| tb | 722.05 | K | Joback Method |
| tc | 963.42 | K | Joback Method |
| tf | 387.31 | K | Joback Method |
| vc | 0.776 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 548.14 | J/mol×K | 722.05 | Joback Method |
| cpg | 564.25 | J/mol×K | 762.28 | Joback Method |
| cpg | 579.06 | J/mol×K | 802.51 | Joback Method |
| cpg | 592.67 | J/mol×K | 842.73 | Joback Method |
| cpg | 605.16 | J/mol×K | 882.96 | Joback Method |
| cpg | 616.63 | J/mol×K | 923.19 | Joback Method |
| cpg | 627.16 | J/mol×K | 963.42 | 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=C1907693&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|---|
| chs: | Standard solid enthalpy of combustion |
| 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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