

# di-p-Anisylideneacetone

|                      |                                                                                                                                                                                                                                                               |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Dianisylideneacetone<br>di(4-Methoxybenzylidene)acetone<br>1,4-Pentadien-3-one, 1,5-bis(p-methoxyphenyl)-<br>1,4-Pentadien-3-one, 1,5-bis(4-methoxyphenyl)-<br>1,5-Bis(p-methoxyphenyl)-3-pentadienone<br>Bis(4-methoxybenzylidene)acetone<br>Dianisalacetone |
| Inchi:               | InChI=1S/C19H18O3/c1-21-18-11-5-15(6-12-18)3-9-17(20)10-4-16-7-13-19(22-2)14-8-16                                                                                                                                                                             |
| InchiKey:            | IOZVKDXPBWBUKY-LQIBPGRFSA-N                                                                                                                                                                                                                                   |
| Formula:             | C19H18O3                                                                                                                                                                                                                                                      |
| SMILES:              | COc1ccc(C=CC(=O)C=Cc2ccc(OC)cc2)cc1                                                                                                                                                                                                                           |
| Mol. weight [g/mol]: | 294.34                                                                                                                                                                                                                                                        |
| CAS:                 | 2051-07-2                                                                                                                                                                                                                                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 136.18  | kJ/mol  | Joback Method  |
| hf            | -127.95 | kJ/mol  | Joback Method  |
| hfus          | 36.65   | kJ/mol  | Joback Method  |
| hvap          | 75.25   | kJ/mol  | Joback Method  |
| log10ws       | -4.71   |         | Crippen Method |
| logp          | 3.999   |         | Crippen Method |
| mcvol         | 235.760 | ml/mol  | McGowan Method |
| pc            | 1928.74 | kPa     | Joback Method  |
| tb            | 804.47  | K       | Joback Method  |
| tc            | 1040.15 | K       | Joback Method  |
| tf            | 466.00  | K       | Joback Method  |
| vc            | 0.885   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 657.13 | J/mol×K | 804.47          | Joback Method |
| cpg           | 721.51 | J/mol×K | 1000.87         | Joback Method |

|       |           |         |         |               |
|-------|-----------|---------|---------|---------------|
| cpg   | 710.69    | J/mol×K | 961.59  | Joback Method |
| cpg   | 698.91    | J/mol×K | 922.31  | Joback Method |
| cpg   | 686.10    | J/mol×K | 883.03  | Joback Method |
| cpg   | 672.20    | J/mol×K | 843.75  | Joback Method |
| cpg   | 731.44    | J/mol×K | 1040.15 | Joback Method |
| dvisc | 0.0000503 | Pa×s    | 804.47  | Joback Method |
| dvisc | 0.0000636 | Pa×s    | 748.06  | Joback Method |
| dvisc | 0.0000836 | Pa×s    | 691.65  | Joback Method |
| dvisc | 0.0001154 | Pa×s    | 635.24  | Joback Method |
| dvisc | 0.0001695 | Pa×s    | 578.82  | Joback Method |
| dvisc | 0.0002706 | Pa×s    | 522.41  | Joback Method |
| dvisc | 0.0004836 | Pa×s    | 466.00  | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051072&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051072&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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