

# 6-Methoxy thymyl tiglate

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C16H22O3/c1-7-11(4)16(17)19-15-8-12(5)14(18-6)9-13(15)10(2)3/h7-10H,1-6H |
| InchiKey:            | LLEOAKBZOLWGPN-YRNVUSSQSA-N                                                       |
| Formula:             | C16H22O3                                                                          |
| SMILES:              | CC=C(C)C(=O)Oc1cc(C)c(OC)cc1C(C)C                                                 |
| Mol. weight [g/mol]: | 262.34                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -102.33 | kJ/mol  | Joback Method  |
| hf            | -446.32 | kJ/mol  | Joback Method  |
| hfus          | 29.41   | kJ/mol  | Joback Method  |
| hvap          | 66.69   | kJ/mol  | Joback Method  |
| log10ws       | -4.68   |         | Crippen Method |
| logp          | 3.999   |         | Crippen Method |
| mcvol         | 221.550 | ml/mol  | McGowan Method |
| pc            | 1774.35 | kPa     | Joback Method  |
| rinpol        | 1859.00 |         | NIST Webbook   |
| rinpol        | 1859.00 |         | NIST Webbook   |
| tb            | 709.41  | K       | Joback Method  |
| tc            | 918.94  | K       | Joback Method  |
| tf            | 394.41  | K       | Joback Method  |
| vc            | 0.841   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 604.48 | J/mol×K | 709.41          | Joback Method |
| cpg           | 620.88 | J/mol×K | 744.33          | Joback Method |
| cpg           | 636.32 | J/mol×K | 779.25          | Joback Method |
| cpg           | 650.82 | J/mol×K | 814.17          | Joback Method |
| cpg           | 664.40 | J/mol×K | 849.10          | Joback Method |
| cpg           | 677.07 | J/mol×K | 884.02          | Joback Method |
| cpg           | 688.85 | J/mol×K | 918.94          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U413805&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U413805&amp;Units=SI</a> |
| <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>                     |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <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>rlnpol:</b>  | Non-polar retention indices                     |
| <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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