

# bornyl benzoate

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C17H22O2/c1-16(2)13-9-10-17(16,3)14(11-13)19-15(18)12-7-5-4-6-8-12/h4-8, |
| InchiKey:            | FLOISDYCXINJOB-KEYYUXOJSA-N                                                       |
| Formula:             | C17H22O2                                                                          |
| SMILES:              | CC1(C)C2CCC1(C)C(OC(=O)c1ccccc1)C2                                                |
| Mol. weight [g/mol]: | 258.36                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 53.75   | kJ/mol  | Joback Method  |
| hf            | -273.24 | kJ/mol  | Joback Method  |
| hfus          | 20.33   | kJ/mol  | Joback Method  |
| hvap          | 61.95   | kJ/mol  | Joback Method  |
| log10ws       | -4.66   |         | Crippen Method |
| logp          | 4.058   |         | Crippen Method |
| mcvol         | 212.350 | ml/mol  | McGowan Method |
| pc            | 2135.43 | kPa     | Joback Method  |
| rinpol        | 1749.00 |         | NIST Webbook   |
| rinpol        | 1749.00 |         | NIST Webbook   |
| rinpol        | 1749.00 |         | NIST Webbook   |
| tb            | 700.22  | K       | Joback Method  |
| tc            | 939.44  | K       | Joback Method  |
| tf            | 451.61  | K       | Joback Method  |
| vc            | 0.803   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 624.43 | J/mol×K | 700.22          | Joback Method |
| cpg           | 644.92 | J/mol×K | 740.09          | Joback Method |
| cpg           | 664.64 | J/mol×K | 779.96          | Joback Method |
| cpg           | 683.94 | J/mol×K | 819.83          | Joback Method |
| cpg           | 703.13 | J/mol×K | 859.70          | Joback Method |
| cpg           | 722.54 | J/mol×K | 899.57          | Joback Method |
| cpg           | 742.50 | J/mol×K | 939.44          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=R204847&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R204847&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpola:</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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