

# Phenylacetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C18H22O2/c1-14(2)10-11-17(12-15(3)4)20-18(19)13-16-8-6-5-7-9-16/h5-9,15, |
| InchiKey:            | KUQMVCQVSLJQDB-UHFFFAOYSA-N   |
| Formula:             | C18H22O2  |
| SMILES:              | <chem>C=C(C)C#CC(CC(C)C)OC(=O)Cc1ccccc1</chem>                                    |
| Mol. weight [g/mol]: | 270.37  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 256.38  | kJ/mol               | Joback Method  |
| hf            | -45.74  | kJ/mol               | Joback Method  |
| hfus          | 32.69   | kJ/mol               | Joback Method  |
| hvap          | 67.88   | kJ/mol               | Joback Method  |
| log10ws       | -4.84   |                      | Crippen Method |
| logp          | 3.767   |                      | Crippen Method |
| mvol          | 235.260 | ml/mol               | McGowan Method |
| pc            | 1816.95 | kPa                  | Joback Method  |
| rinpol        | 1826.30 |                      | NIST Webbook   |
| tb            | 718.89  | K                    | Joback Method  |
| tc            | 942.50  | K                    | Joback Method  |
| tf            | 451.58  | K                    | Joback Method  |
| vc            | 0.891   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 641.70 | J/mol×K | 718.89          | Joback Method |
| cpg           | 659.40 | J/mol×K | 756.16          | Joback Method |
| cpg           | 675.92 | J/mol×K | 793.43          | Joback Method |
| cpg           | 691.29 | J/mol×K | 830.69          | Joback Method |
| cpg           | 705.57 | J/mol×K | 867.96          | Joback Method |
| cpg           | 718.81 | J/mol×K | 905.23          | Joback Method |
| cpg           | 731.06 | J/mol×K | 942.50          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U292535&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292535&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>                                     |

# 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>rinpol:</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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