

# 2,3,4-Trifluorobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

**Inchi:** InChI=1S/C17H17F3O2/c1-10(2)5-6-12(9-11(3)4)22-17(21)13-7-8-14(18)16(20)15(13)19  
**InchiKey:** CVPJVVUHNCAABL-UHFFFAOYSA-N  
**Formula:** C17H17F3O2  
**SMILES:** C=C(C)C#CC(CC(C)C)OC(=O)c1ccc(F)c(F)c1F  
**Mol. weight [g/mol]:** 310.31

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -365.36 | kJ/mol  | Joback Method  |
| hf            | -647.84 | kJ/mol  | Joback Method  |
| hfus          | 38.17   | kJ/mol  | Joback Method  |
| hvap          | 65.19   | kJ/mol  | Joback Method  |
| log10ws       | -5.99   |         | Crippen Method |
| logp          | 4.255   |         | Crippen Method |
| mcvol         | 226.480 | ml/mol  | McGowan Method |
| pc            | 1693.51 | kPa     | Joback Method  |
| rinpol        | 1743.30 |         | NIST Webbook   |
| tb            | 708.76  | K       | Joback Method  |
| tc            | 912.31  | K       | Joback Method  |
| tf            | 479.64  | K       | Joback Method  |
| vc            | 0.889   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 608.78 | J/mol×K | 708.76          | Joback Method |
| cpg           | 623.60 | J/mol×K | 742.68          | Joback Method |
| cpg           | 637.52 | J/mol×K | 776.61          | Joback Method |
| cpg           | 650.58 | J/mol×K | 810.53          | Joback Method |
| cpg           | 662.80 | J/mol×K | 844.46          | Joback Method |
| cpg           | 674.20 | J/mol×K | 878.38          | Joback Method |
| cpg           | 684.79 | J/mol×K | 912.31          | 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=U292557&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292557&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>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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