# 3-Trifluoromethylbenzoic acid, 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C17H19F3O2/c1-4-5-9-15(10-12(2)3)22-16(21)13-7-6-8-14(11-13)17(18,19)20

**InchiKey:** UGULVPZUNSSSBY-UHFFFAOYSA-N

**Formula:** C17H19F3O2

**SMILES:** CCC#CC(CC(C)C)OC(=O)c1cccc(C(F)(F)F)c1

**Mol. weight [g/mol]:** 312.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -422.55 | kJ/mol | Joback Method |
| hf | -749.29 | kJ/mol | Joback Method |
| hfus | 34.13 | kJ/mol | Joback Method |
| hvap | 63.16 | kJ/mol | Joback Method |
| log10ws | -5.83 | | Crippen Method |
| logp | 4.690 | | Crippen Method |
| mcvol | 230.780 | ml/mol | McGowan Method |
| pc | 1696.30 | kPa | Joback Method |
| rinpol | 1651.00 | | NIST Webbook |
| rinpol | 1651.00 | | NIST Webbook |
| tb | 699.01 | K | Joback Method |
| tc | 904.33 | K | Joback Method |
| tf | 472.74 | K | Joback Method |
| vc | 0.896 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 637.00 | J/mol×K | 699.01 | Joback Method |
| cpg | 652.91 | J/mol×K | 733.23 | Joback Method |
| cpg | 667.77 | J/mol×K | 767.45 | Joback Method |
| cpg | 681.65 | J/mol×K | 801.67 | Joback Method |
| cpg | 694.58 | J/mol×K | 835.89 | Joback Method |
| cpg | 706.62 | J/mol×K | 870.11 | Joback Method |
| cpg | 717.80 | J/mol×K | 904.33 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U299324&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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