# o-anisic acid, 2-methyloct-5-yn-4-yl ester

**Inchi:** InChI=1S/C17H22O3/c1-5-6-9-14(12-13(2)3)20-17(18)15-10-7-8-11-16(15)19-4/h7-8,10-
**InchiKey:** DKGCROILSHCXBK-UHFFFAOYSA-N
**Formula:** C17H22O3
**SMILES:** CCC#CC(CC(C)C)OC(=O)c1ccccc1OC
**Mol. weight [g/mol]:** 274.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -320.62 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 33.49 | kJ/mol | Joback Method |
| hvap | 84.45 | kJ/mol | Cheméo Relay (1.0) |
| log10ws | -4.53 | | Cheméo Relay (1.0) |
| logp | 3.680 | | Crippen Method |
| mcvol | 231.340 | ml/mol | McGowan Method |
| rinpol | 1944.40 | | NIST Webbook |
| rinpol | 1944.40 | | NIST Webbook |
| tb | 583.39 | K | Cheméo Relay (1.0) |
| tf | 275.00 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 638.93 | J/mol×K | 726.85 | Joback Method |
| cpg | 656.04 | J/mol×K | 763.23 | Joback Method |
| cpg | 672.03 | J/mol×K | 799.60 | Joback Method |
| cpg | 686.92 | J/mol×K | 835.98 | Joback Method |
| cpg | 700.73 | J/mol×K | 872.36 | Joback Method |
| cpg | 713.46 | J/mol×K | 908.73 | Joback Method |
| cpg | 725.13 | J/mol×K | 945.11 | Joback Method |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U292575&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |