# o-Anisic acid, 2-(1-adamantyl)ethyl ester

**Inchi:** InChI=1S/C20H26O3/c1-22-18-5-3-2-4-17(18)19(21)23-7-6-20-11-14-8-15(12-20)10-16(9
**InchiKey:** IFNXVXHTDVOPQW-UHFFFAOYSA-N
**Formula:** C20H26O3
**SMILES:** COc1ccccc1C(=O)OCCC12CC3CC(CC(C3)C1)C2
**Mol. weight [g/mol]:** 314.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 38.33 | kJ/mol | Joback Method |
| hf | -400.95 | kJ/mol | Joback Method |
| hfus | 32.26 | kJ/mol | Joback Method |
| hvap | 73.07 | kJ/mol | Joback Method |
| log10ws | -5.16 | | Crippen Method |
| logp | 4.459 | | Crippen Method |
| mcvol | 249.630 | ml/mol | McGowan Method |
| pc | 1786.37 | kPa | Joback Method |
| rinpol | 2527.00 | | NIST Webbook |
| tb | 807.43 | K | Joback Method |
| tc | 1037.73 | K | Joback Method |
| tf | 518.45 | K | Joback Method |
| vc | 0.950 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 811.72 | J/mol×K | 807.43 | Joback Method |
| cpg | 832.39 | J/mol×K | 845.81 | Joback Method |
| cpg | 852.36 | J/mol×K | 884.20 | Joback Method |
| cpg | 871.85 | J/mol×K | 922.58 | Joback Method |
| cpg | 891.07 | J/mol×K | 960.96 | Joback Method |
| cpg | 910.25 | J/mol×K | 999.34 | Joback Method |
| cpg | 929.61 | J/mol×K | 1037.73 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=U299950&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |