# 1,4-ANDROSTADIENE-3,11,17-TRIONE

**Other names:** 1,4-Androstadiene-3,11,17-trione
**Inchi:** InChI=1S/C19H22O3/c1-18-8-7-12(20)9-11(18)3-4-13-14-5-6-16(22)19(14,2)10-15(21)17
**InchiKey:** RZACPWSZIQKVDY-GFPCFBFFSA-N
**Formula:** C19H22O3
**SMILES:** C[C@]12C=CC(=O)C=C1CC[C@@H]1[C@@H]2C(=O)C[C@]2(C)C(=O)CC[C@@H]12
**Mol. weight [g/mol]:** 298.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hfus | 16.07 | kJ/mol | Joback Method |
| log10ws | -3.84 | | Cheméo Relay (1.0) |
| logp | 3.042 | | Crippen Method |
| mcvol | 231.240 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 814.88 | J/mol×K | 885.00 | Joback Method |
| cpg | 841.05 | J/mol×K | 931.20 | Joback Method |
| cpg | 867.40 | J/mol×K | 977.40 | Joback Method |
| cpg | 894.32 | J/mol×K | 1023.60 | Joback Method |
| cpg | 922.22 | J/mol×K | 1069.80 | Joback Method |
| cpg | 951.49 | J/mol×K | 1116.00 | Joback Method |
| cpg | 982.54 | J/mol×K | 1162.20 | Joback Method |

## Sources

**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C7738934&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

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

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |