

Androst-4-en-3-one, 4-chloro-17-hydroxy-, (17«beta»)-

Other names:

Clostebol Acetate
4-Chloro-17«beta»-hydroxyandrost-4-en-3-one
4-Chlorotestosterone
Clostebol
4-Chloro-17beta-hydroxyandrost-4-en-3-one

Inchi:

InChI=1S/C19H27ClO2/c1-18-10-8-15(21)17(20)14(18)4-3-11-12-5-6-16(22)19(12,2)9-7-

InchiKey:

KCZCIYZKSLNNH-MQPPDSCVSA-N

Formula:

C19H27ClO2

SMILES:

CC12CCC(=O)C(Cl)=C1CCC1C2CCC2(C)C(O)CCC12

Mol. weight [g/mol]:

322.87

CAS:

1093-58-9

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 4.56 | kJ/mol | Joback Method |
| hf | -456.12 | kJ/mol | Joback Method |
| hfus | 24.79 | kJ/mol | Joback Method |
| hvap | 82.41 | kJ/mol | Joback Method |
| log10ws | -5.30 | | Crippen Method |
| logp | 4.446 | | Crippen Method |
| mcvol | 250.510 | ml/mol | McGowan Method |
| pc | 1928.74 | kPa | Joback Method |
| tb | 880.12 | K | Joback Method |
| tc | 1119.74 | K | Joback Method |
| tf | 582.13 | K | Joback Method |
| vc | 0.943 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 871.10 | J/mol×K | 880.12 | Joback Method |
| cpg | 894.96 | J/mol×K | 920.06 | Joback Method |
| cpg | 919.16 | J/mol×K | 959.99 | Joback Method |
| cpg | 944.02 | J/mol×K | 999.93 | Joback Method |

| | | | | |
|-----|---------|---------|---------|---------------|
| cpg | 969.90 | J/mol×K | 1039.86 | Joback Method |
| cpg | 997.10 | J/mol×K | 1079.80 | Joback Method |
| cpg | 1025.96 | J/mol×K | 1119.74 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C1093589&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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