# atisirene

**Inchi:** InChI=1S/C21H36/c1-18(2)9-6-10-20(5)16(18)8-12-21-11-7-15(13-17(20)21)19(3,4)14-21
**InchiKey:** OFOGPDDZNWXWEO-PWLWMKPSSA-N
**Formula:** C21H36
**SMILES:** CC1(C)CC23CCC1CC2C1(C)CCCC(C)(C)C1CC3
**Mol. weight [g/mol]:** 288.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 275.45 | kJ/mol | Joback Method |
| hf | -210.27 | kJ/mol | Joback Method |
| hfus | 12.31 | kJ/mol | Joback Method |
| hvap | 57.15 | kJ/mol | Joback Method |
| log10ws | -6.50 | | Crippen Method |
| logp | 6.445 | | Crippen Method |
| mcvol | 263.310 | ml/mol | McGowan Method |
| pc | 1558.58 | kPa | Joback Method |
| rinpol | 2054.00 | | NIST Webbook |
| tb | 710.87 | K | Joback Method |
| tc | 954.62 | K | Joback Method |
| tf | 466.99 | K | Joback Method |
| vc | 0.997 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 850.56 | J/mol×K | 710.87 | Joback Method |
| cpg | 880.31 | J/mol×K | 751.50 | Joback Method |
| cpg | 909.67 | J/mol×K | 792.12 | Joback Method |
| cpg | 939.30 | J/mol×K | 832.75 | Joback Method |
| cpg | 969.84 | J/mol×K | 873.37 | Joback Method |
| cpg | 1001.96 | J/mol×K | 914.00 | Joback Method |
| cpg | 1036.31 | J/mol×K | 954.62 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R221293&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |