# (6Z,8E)-4,6,8-megastigmatrien-3-one

**Inchi:** InChI=1S/C13H18O/c1-5-6-7-12-10(2)8-11(14)9-13(12,3)4/h5-8H,9H2,1-4H3/b6-5+,12-7
**InchiKey:** CBQXHTWJSZXYSK-DFTQQVSXSA-N
**Formula:** C13H18O
**SMILES:** CC=CC=C1C(C)=CC(=O)CC1(C)C
**Mol. weight [g/mol]:** 190.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 100.96 | kJ/mol | Joback Method |
| hf | -140.23 | kJ/mol | Joback Method |
| hfus | 15.83 | kJ/mol | Joback Method |
| hvap | 49.76 | kJ/mol | Joback Method |
| log10ws | -3.76 | | Crippen Method |
| logp | 3.434 | | Crippen Method |
| mcvol | 171.840 | ml/mol | McGowan Method |
| pc | 2313.61 | kPa | Joback Method |
| rinpol | 1534.00 | | NIST Webbook |
| rinpol | 1534.00 | | NIST Webbook |
| ripol | 2193.00 | | NIST Webbook |
| tb | 599.39 | K | Joback Method |
| tc | 830.25 | K | Joback Method |
| tf | 354.33 | K | Joback Method |
| vc | 0.650 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 427.35 | J/mol×K | 599.39 | Joback Method |
| cpg | 445.16 | J/mol×K | 637.87 | Joback Method |
| cpg | 462.00 | J/mol×K | 676.34 | Joback Method |
| cpg | 478.00 | J/mol×K | 714.82 | Joback Method |
| cpg | 493.28 | J/mol×K | 753.29 | Joback Method |
| cpg | 507.98 | J/mol×K | 791.77 | Joback Method |
| cpg | 522.21 | J/mol×K | 830.25 | 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=R288885&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |