

Stigmastane-3,6-dione, (5«alpha»)-

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|-----------------------------|--|
| Other names: | 5«alpha»-Stigmastane-3,6-dione 5«alpha»-Stigmast-3,6-dione |
| Inchi: | InChI=1S/C29H48O2/c1-7-20(18(2)3)9-8-19(4)23-10-11-24-22-17-27(31)26-16-21(30)12 |
| InchiKey: | HMMVBUVVQLUGQA-QSWZYIJZSA-N |
| Formula: | C29H48O2 |
| SMILES: | CCC(CCC(C)C1CCC2C3CC(=O)C4CC(=O)CCC4(C)C3CCC12C)C(C)C |
| Mol. weight [g/mol]: | 428.69 |
| CAS: | 22149-69-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 89.19 | kJ/mol | Joback Method |
| hf | -703.27 | kJ/mol | Joback Method |
| hfus | 31.97 | kJ/mol | Joback Method |
| hvap | 84.76 | kJ/mol | Joback Method |
| log10ws | -7.68 | | Crippen Method |
| logp | 7.492 | | Crippen Method |
| mcvol | 379.170 | ml/mol | McGowan Method |
| pc | 934.06 | kPa | Joback Method |
| rinpol | 3601.00 | | NIST Webbook |
| rinpol | 3601.00 | | NIST Webbook |
| tb | 1032.02 | K | Joback Method |
| tc | 1274.97 | K | Joback Method |
| tf | 597.27 | K | Joback Method |
| vc | 1.437 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1505.04 | J/molxK | 1032.02 | Joback Method |
| cpg | 1539.65 | J/molxK | 1072.51 | Joback Method |
| cpg | 1574.79 | J/molxK | 1113.00 | Joback Method |
| cpg | 1610.80 | J/molxK | 1153.50 | Joback Method |
| cpg | 1648.03 | J/molxK | 1193.99 | Joback Method |

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|-----|---------|---------|---------|---------------|
| cpg | 1686.83 | J/mol×K | 1234.48 | Joback Method |
| cpg | 1727.53 | J/mol×K | 1274.97 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C22149695&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| rinpolar: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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