# Stigmasta-7,25-dien-3-ol, (3«beta»,5«alpha»)-

| | |
|---|---|
| **Other names:** | 5«alpha»-Stigmasta-7,25-dien-3«beta»-ol |
| | «delta»7,25-Stigmastadienol |
| | 24-Ethyl-5-«alpha»-cholest-7,25-dien-3-«beta»-ol |
| | 24«beta»-Ethyl-5«alpha»-cholesta-7,25-dien-3«beta»-ol |
| | Stigmasta-7,25(27)-dien-3-ol, (3«beta»,5«alpha»)- |
| **Inchi:** | InChI=1S/C29H48O/c1-7-21(19(2)3)9-8-20(4)25-12-13-26-24-11-10-22-18-23(30)14-16-2 |
| **InchiKey:** | CMQUSRGUOMCHOZ-UHFFFAOYSA-N |
| **Formula:** | C29H48O |
| **SMILES:** | C=C(C)C(CC)CCC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C |
| **Mol. weight [g/mol]:** | 412.69 |
| **CAS:** | 6785-58-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 299.61 | kJ/mol | Joback Method |
| hf | -412.87 | kJ/mol | Joback Method |
| hfus | 38.81 | kJ/mol | Joback Method |
| hvap | 93.70 | kJ/mol | Joback Method |
| log10ws | -8.69 | | Crippen Method |
| logp | 7.945 | | Crippen Method |
| mcvol | 373.300 | ml/mol | McGowan Method |
| pc | 982.69 | kPa | Joback Method |
| rinpol | 3325.00 | | NIST Webbook |
| tb | 989.70 | K | Joback Method |
| tc | 1215.93 | K | Joback Method |
| tf | 534.21 | K | Joback Method |
| vc | 1.415 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1425.71 | J/mol×K | 989.70 | Joback Method |
| cpg | 1458.39 | J/mol×K | 1027.41 | Joback Method |
| cpg | 1491.94 | J/mol×K | 1065.11 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 1526.71 | J/mol×K | 1102.82 | Joback Method |
| cpg | 1563.07 | J/mol×K | 1140.52 | Joback Method |
| cpg | 1601.37 | J/mol×K | 1178.23 | Joback Method |
| cpg | 1641.95 | J/mol×K | 1215.93 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=C6785586&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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