# Tigogenin

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|---|---|
| **Other names:** | Spirostan-3-ol, (3«beta»,5«alpha»,25R)-<br>5«alpha»-Spirostan-3«beta»-ol, (25R)-<br>(25R)-5«alpha»-Spirostan-3«beta»-ol<br>Spiro[8H-naphth[2',1':4,5]indeno[2,1-b]furan-8,2'-[2H]pyran], spirostan-3-ol deriv.<br>(5«alpha»,25R)-spirostan-3«beta»-ol |
| **Inchi:** | InChI=1S/C27H44O3/c1-16-7-12-27(29-15-16)17(2)24-23(30-27)14-22-20-6-5-18-13-19( |
| **InchiKey:** | GMBQZIIUCVWOCD-PODJHBEMSA-N |
| **Formula:** | C27H44O3 |
| **SMILES:** | CC1CCC2(OC1)OC1CC3C4CCC5CC(O)CCC5(C)C4CCC3(C)C1C2C |
| **Mol. weight [g/mol]:** | 416.64 |
| **CAS:** | 77-60-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 84.47 | kJ/mol | Joback Method |
| hf | -699.48 | kJ/mol | Joback Method |
| hfus | 47.37 | kJ/mol | Joback Method |
| hvap | 96.77 | kJ/mol | Joback Method |
| log10ws | -6.59 | | Crippen Method |
| logp | 5.794 | | Crippen Method |
| mcvol | 343.740 | ml/mol | McGowan Method |
| pc | 1236.35 | kPa | Joback Method |
| rinpol | 3260.00 | | NIST Webbook |
| rinpol | 3232.00 | | NIST Webbook |
| tb | 1006.27 | K | Joback Method |
| tc | 1247.23 | K | Joback Method |
| tf | 477.90 ± 5.00 | K | NIST Webbook |
| vc | 1.282 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1428.95 | J/mol×K | 1006.27 | Joback Method |
| cpg | 1469.35 | J/mol×K | 1046.43 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 1512.10 | J/mol×K | 1086.59 | Joback Method |
| cpg | 1557.75 | J/mol×K | 1126.75 | Joback Method |
| cpg | 1606.85 | J/mol×K | 1166.91 | Joback Method |
| cpg | 1659.94 | J/mol×K | 1207.07 | Joback Method |
| cpg | 1717.59 | J/mol×K | 1247.23 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C77601&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |

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