

31-Nor-7-lanosterol acetate

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| Inchi: | InChI=1S/C31H52O2/c1-9-10-11-12-21(2)23-15-19-31(8)25-13-14-26-28(4,5)27(33-22(3 |
| InchiKey: | KAQDYZSKYROZFD-IMQMZZFDSA-N |
| Formula: | C31H52O2 |
| SMILES: | CCCCC(C)C1CCC2(C)C3=CCC4C(C)(C)C(OC(C)=O)CCC4(C)C3CCC12C |
| Mol. weight [g/mol]: | 456.74 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 123.81 | kJ/mol | Joback Method |
| hf | -646.94 | kJ/mol | Joback Method |
| hfus | 37.27 | kJ/mol | Joback Method |
| hvap | 88.99 | kJ/mol | Joback Method |
| log10ws | -9.27 | | Crippen Method |
| logp | 8.740 | | Crippen Method |
| mcvol | 407.350 | ml/mol | McGowan Method |
| pc | 851.97 | kPa | Joback Method |
| rinpola | 3286.00 | | NIST Webbook |
| rinpola | 3286.00 | | NIST Webbook |
| tb | 1019.26 | K | Joback Method |
| tc | 1254.31 | K | Joback Method |
| tf | 642.37 | K | Joback Method |
| vc | 1.552 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1598.35 | J/molxK | 1019.26 | Joback Method |
| cpg | 1645.55 | J/molxK | 1058.43 | Joback Method |
| cpg | 1696.03 | J/molxK | 1097.61 | Joback Method |
| cpg | 1750.35 | J/molxK | 1136.78 | Joback Method |
| cpg | 1809.09 | J/molxK | 1175.96 | Joback Method |
| cpg | 1872.84 | J/molxK | 1215.13 | Joback Method |
| cpg | 1942.16 | J/molxK | 1254.31 | 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=R110628&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

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 |
| hvp: | 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 |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/64-454-7/31-Nor-7-lanosterol-acetate.pdf>

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