# Methyl 5-«beta»-cholan-12-«alpha»-ol-3-one-24-oate

**Inchi:** InChI=1S/C25H40O4/c1-15(5-10-23(28)29-4)19-8-9-20-18-7-6-16-13-17(26)11-12-24(16

**InchiKey:** LOJPGRHPJBGMMF-ZHVGCCDGSA-N

**Formula:** C25H40O4

**SMILES:** COC(=O)CCC(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CC(O)C12C

**Mol. weight [g/mol]:** 404.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -195.47 | kJ/mol | Joback Method |
| hf | -889.82 | kJ/mol | Joback Method |
| hfus | 37.10 | kJ/mol | Joback Method |
| hvap | 97.91 | kJ/mol | Joback Method |
| log10ws | -5.45 | | Crippen Method |
| logp | 4.774 | | Crippen Method |
| mcvol | 334.550 | ml/mol | McGowan Method |
| pc | 1245.09 | kPa | Joback Method |
| rinpol | 3223.00 | | NIST Webbook |
| tb | 1037.36 | K | Joback Method |
| tc | 1274.40 | K | Joback Method |
| tf | 642.71 | K | Joback Method |
| vc | 1.260 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1332.80 | J/mol×K | 1037.36 | Joback Method |
| cpg | 1363.62 | J/mol×K | 1076.87 | Joback Method |
| cpg | 1395.25 | J/mol×K | 1116.37 | Joback Method |
| cpg | 1427.99 | J/mol×K | 1155.88 | Joback Method |
| cpg | 1462.15 | J/mol×K | 1195.39 | Joback Method |
| cpg | 1498.07 | J/mol×K | 1234.90 | Joback Method |
| cpg | 1536.04 | J/mol×K | 1274.40 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R215768&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

| | |
|---|---|
| **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 |