

Cholan-24-oic acid, 7-hydroxy-3-oxo-, methyl ester, (5«beta»,7«alpha»)-

Other names:

5«beta»-Cholan-24-oic acid, 7«alpha»-hydroxy-3-oxo-, methyl ester

Methyl 7-hydroxy-3-oxocholan-24-oate, (5«beta»,7«alpha»)-

Methyl 5-«beta»-cholan-7-«alpha»-ol-3-one-24-oate

Inchi: InChI=1S/C25H40O4/c1-15(5-8-22(28)29-4)18-6-7-19-23-20(10-12-25(18,19)3)24(2)11-9

InchiKey: XHRLTYUHWGHDCJ-HVTKZUMLSA-N

Formula: C25H40O4

SMILES: COC(=O)CCC(C)C1CCC2C3C(O)CC4CC(=O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 404.58

CAS: 14773-00-3

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 | 3258.00 | | NIST Webbook |
| rinpol | 3258.00 | | 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/molxK | 1037.36 | Joback Method |
| cpg | 1363.62 | J/molxK | 1076.87 | Joback Method |
| cpg | 1395.25 | J/molxK | 1116.37 | Joback Method |
| cpg | 1427.99 | J/molxK | 1155.88 | Joback Method |

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|-----|---------|---------|---------|---------------|
| 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=C14773003&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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 |
| hvp: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mvol: | 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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