

syn-4-cholesten-3-one, methyloxime derivative

Inchi: InChI=1S/C28H47NO/c1-19(2)8-7-9-20(3)24-12-13-25-23-11-10-21-18-22(29-30-6)14-16
InchiKey: ANJYUACJDKITGZ-NXRNSRJBSA-N
Formula: C28H47NO
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(C(C)CCCC(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]: 413.68

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -426.49 | kJ/mol | Joback Method |
| hvap | 82.25 | kJ/mol | Joback Method |
| log10ws | -8.28 | | Crippen Method |
| logp | 8.030 | | Crippen Method |
| mcvol | 369.190 | ml/mol | McGowan Method |
| pc | 893.73 | kPa | Joback Method |
| rinpola | 3152.00 | | NIST Webbook |
| rinpola | 3152.00 | | NIST Webbook |
| tb | 984.33 | K | Joback Method |
| tc | 1217.74 | K | Joback Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R417593&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

Legend

hf: Enthalpy of formation 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 |

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