

3Beta-hydroxy-16,17-secoestra-5(10),6,8-trien-17-

Inchi:
acid

InChI=1S/C18H24O3/c1-3-16-15-6-4-11-10-12(19)5-7-13(11)14(15)8-9-18(16,2)17(20)21

InchiKey:

UYDPGFTYMHWMBX-UHFFFAOYSA-N

Formula:

C18H24O3

SMILES:

CCC1c2ccc3c(c2CCC1(C)C(=O)O)CCC(O)C3

Mol. weight [g/mol]:

288.38

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -134.26 | kJ/mol | Joback Method |
| hf | -501.59 | kJ/mol | Joback Method |
| hfus | 31.87 | kJ/mol | Joback Method |
| hvap | 98.74 | kJ/mol | Joback Method |
| log10ws | -4.34 | | Crippen Method |
| logp | 3.067 | | Crippen Method |
| mcvol | 232.310 | ml/mol | McGowan Method |
| pc | 2287.14 | kPa | Joback Method |
| tb | 908.68 | K | Joback Method |
| tc | 1125.44 | K | Joback Method |
| tf | 576.67 | K | Joback Method |
| vc | 0.875 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 781.94 | J/molxK | 908.68 | Joback Method |
| cpg | 798.50 | J/molxK | 944.81 | Joback Method |
| cpg | 814.98 | J/molxK | 980.93 | Joback Method |
| cpg | 831.55 | J/molxK | 1017.06 | Joback Method |
| cpg | 848.37 | J/molxK | 1053.19 | Joback Method |
| cpg | 865.60 | J/molxK | 1089.32 | Joback Method |
| cpg | 883.40 | J/molxK | 1125.44 | 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=B6005484&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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