

# 3,13Alpha-dihydroxy-13,17-secoestra-1,3,5(10),6,8

Inchi:  
acid

InChI=1S/C18H20O4/c1-18(22)9-8-14-13-5-3-12(19)10-11(13)2-4-15(14)16(18)6-7-17(20)

InchiKey:

SEMJUDNMZYNLQ-UHFFFAOYSA-N

Formula:

C18H20O4

SMILES:

CC1(O)CCc2c(ccc3cc(O)ccc23)C1CCC(=O)O

Mol. weight [g/mol]:

300.35

CAS:

133372-01-7

## Physical Properties

Property code	Value	Unit	Source
gf	-221.25	kJ/mol	Joback Method
hf	-543.00	kJ/mol	Joback Method
hfus	39.02	kJ/mol	Joback Method
hvap	112.64	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.191		Crippen Method
mcvol	229.580	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	992.29	K	Joback Method
tc	1222.49	K	Joback Method
tf	694.15	K	Joback Method
vc	0.814	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.30	J/molxK	992.29	Joback Method
cpg	791.38	J/molxK	1030.66	Joback Method
cpg	810.52	J/molxK	1069.02	Joback Method
cpg	830.96	J/molxK	1107.39	Joback Method
cpg	852.95	J/molxK	1145.76	Joback Method
cpg	876.76	J/molxK	1184.13	Joback Method
cpg	902.62	J/molxK	1222.49	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C133372017&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C133372017&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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