3-Hydroxy-16,17-secoestra-1,3,5(10)-triene=16,17-acid

Inchi: InChI=1S/C18H22O5/c1-18(17(22)23)7-6-13-12-5-3-11(19)8-10(12)2-4-14(13)15(18)9-16

InchiKey: AFTZJBUXQQADGN-UHFFFAOYSA-N

Formula: C18H22O5

SMILES: CC1(C(=O)O)CCC2c3ccc(O)cc3CCC2C1CC(=O)O

Mol. weight [g/mol]: 318.36

Physical Properties

Property code	Value	Unit	Source
gf	-406.25	kJ/mol	Joback Method
hf	-788.88	kJ/mol	Joback Method
hfus	41.10	kJ/mol	Joback Method
hvap	116.86	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.014		Crippen Method
mcvol	239.750	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	1028.54	K	Joback Method
tc	1263.57	K	Joback Method
tf	709.04	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.80	J/mol×K	1028.54	Joback Method
cpg	881.59	J/mol×K	1067.71	Joback Method
cpg	902.41	J/mol×K	1106.88	Joback Method
cpg	924.50	J/mol×K	1146.05	Joback Method
cpg	948.14	J/mol×K	1185.22	Joback Method
cpg	973.57	J/mol×K	1224.40	Joback Method
cpg	1001.06	J/mol×K	1263.57	Joback Method

Sources

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=B6005477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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