3,13Alpha-dihydroxy-13,17-secoestra-1,3,5(10)-tri
acid

Inchi: InChI=1S/C18H24O4/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: IYPKGDXFMKJBEI-UHFFFAOYSA-N

Formula: C18H24O4

SMILES: CC1(O)CCC2c3ccc(O)cc3CCC2C1CCC(=O)O

Mol. weight [g/mol]: 304.38

CAS: 133372-02-8

Physical Properties

Property code	Value	Unit	Source
gf	-277.33	kJ/mol	Joback Method
hf	-676.30	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	110.12	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.064		Crippen Method
mcvol	238.180	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	974.67	K	Joback Method
tc	1200.91	K	Joback Method
tf	659.11	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.32	J/mol×K	974.67	Joback Method
cpg	865.08	J/mol×K	1012.38	Joback Method
cpg	884.47	J/mol×K	1050.08	Joback Method
cpg	904.73	J/mol×K	1087.79	Joback Method
cpg	926.09	J/mol×K	1125.50	Joback Method
cpg	948.78	J/mol×K	1163.21	Joback Method
cpg	973.05	J/mol×K	1200.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C133372028&Units=SI

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