3-Hydroxyestra-1,3,5(10)-triene-16,17-dione

Inchi: InChI=1S/C18H20O3/c1-18-7-6-13-12-5-3-11(19)8-10(12)2-4-14(13)15(18)9-16(20)17(18
InchiKey: ANPHVANSJXDRTP-UHFFFAOYSA-N
Formula: C18H20O3
SMILES: CC12CCC3c4ccc(O)cc4CCC3C1CC(=O)C2=O
Mol. weight [g/mol]: 284.35
CAS: 1228-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-51.49	kJ/mol	Joback Method
hf	-441.52	kJ/mol	Joback Method
hfus	25.81	kJ/mol	Joback Method
hvap	78.73	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.996		Crippen Method
mcvol	217.150	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	883.49	K	Joback Method
tc	1156.06	K	Joback Method
tf	646.16	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.34	J/mol×K	883.49	Joback Method
cpg	769.96	J/mol×K	928.92	Joback Method
cpg	791.54	J/mol×K	974.35	Joback Method
cpg	813.43	J/mol×K	1019.77	Joback Method
cpg	835.98	J/mol×K	1065.20	Joback Method
cpg	859.54	J/mol×K	1110.63	Joback Method
cpg	884.45	J/mol×K	1156.06	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=C1228735&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