3-Hydroxyestra-2,5(10)-diene-1,4,17-trione

Inchi: InChI=1S/C18H20O4/c1-18-7-6-10-9(12(18)4-5-15(18)21)2-3-11-16(10)13(19)8-14(20)17

InchiKey: SDARQPHJTCICSI-UHFFFAOYSA-N

Formula: C18H20O4

SMILES: CC12CCC3C4=C(CCC3C1CCC2=O)C(=O)C(O)=CC4=O

Mol. weight [g/mol]: 300.35

CAS: 94996-48-2

Physical Properties

Property code	Value	Unit	Source
gf	-195.87	kJ/mol	Joback Method
hf	-623.39	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.682		Crippen Method
mcvol	223.020	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	968.69	K	Joback Method
tc	1222.95	K	Joback Method
tf	675.24	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.48	J/mol×K	968.69	Joback Method
cpg	832.36	J/mol×K	1011.07	Joback Method
cpg	850.74	J/mol×K	1053.44	Joback Method
cpg	868.80	J/mol×K	1095.82	Joback Method
cpg	886.68	J/mol×K	1138.20	Joback Method
cpg	904.56	J/mol×K	1180.57	Joback Method
cpg	922.58	J/mol×K	1222.95	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=C94996482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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