3-Ethoxycarbonyl-17-oxaestra-1,3,5(10)-trien-16-o

Inchi: InChI=1S/C20H24O4/c1-3-23-19(22)13-5-6-14-12(10-13)4-7-16-15(14)8-9-20(2)17(16)11
InchiKey: ISAOGXCREJVTNK-UHFFFAOYSA-N
Formula: C20H24O4
SMILES: CCOC(=O)c1ccc2c(c1)CCC1C2CCC2(C)OC(=O)CC12
Mol. weight [g/mol]: 328.40

Physical Properties

Property code	Value	Unit	Source
gf	-87.11	kJ/mol	Joback Method
hf	-556.06	kJ/mol	Joback Method
hfus	36.07	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.625		Crippen Method
mcvol	251.200	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
tb	889.03	K	Joback Method
tc	1135.54	K	Joback Method
tf	600.01	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.00	J/mol×K	889.03	Joback Method
cpg	875.57	J/mol×K	930.12	Joback Method
cpg	895.61	J/mol×K	971.20	Joback Method
cpg	915.36	J/mol×K	1012.29	Joback Method
cpg	935.02	J/mol×K	1053.37	Joback Method
cpg	954.81	J/mol×K	1094.46	Joback Method
cpg	974.96	J/mol×K	1135.54	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=B6005486&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