3-Acetoxy-17alpha-ethylestra-1,3,5(10),6,8-pentae

Inchi: InChI=1S/C22H26O3/c1-4-22(24)12-10-20-19-7-5-15-13-16(25-14(2)23)6-8-17(15)18(19
InchiKey: YQEMHVRYFAVXBT-UHFFFAOYSA-N
Formula: C22H26O3
SMILES: CCC1(O)CCC2c3ccc4cc(OC(C)=O)ccc4c3CCC21C
Mol. weight [g/mol]: 338.44
CAS: 133070-71-0

Physical Properties

Property code	Value	Unit	Source
gf	44.50	kJ/mol	Joback Method
hf	-351.67	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	93.69	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	4.736		Crippen Method
mcvol	269.210	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
tb	945.39	K	Joback Method
tc	1177.95	K	Joback Method
tf	643.28	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.37	J/mol×K	945.39	Joback Method
cpg	934.76	J/mol×K	984.15	Joback Method
cpg	959.37	J/mol×K	1022.91	Joback Method
cpg	985.53	J/mol×K	1061.67	Joback Method
cpg	1013.59	J/mol×K	1100.43	Joback Method
cpg	1043.87	J/mol×K	1139.19	Joback Method
cpg	1076.71	J/mol×K	1177.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C133070710&Units=SI
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

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