(-)-3-Menthoxyacetoxy-(+)-estra-1,3,5(10),6,8-pent

Inchi: InChI=1S/C30H38O4/c1-18(2)22-8-5-19(3)15-27(22)33-17-29(32)34-21-7-10-23-20(16-2
InchiKey: JIPJTPKULQRHGR-BJEUKTRSSA-N
Formula: C30H38O4
SMILES: CC1CCC(C(C)C)C(OCC(=O)Oc2ccc3c4c(ccc3c2)C2CCC(=O)C2(C)CC4)C1
Mol. weight [g/mol]: 462.62

Physical Properties

Property code	Value	Unit	Source
gf	40.88	kJ/mol	Joback Method
hf	-621.02	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	102.36	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	6.622		Crippen Method
mcvol	372.640	ml/mol	McGowan Method
pc	1092.10	kPa	Joback Method
tb	1140.69	K	Joback Method
tc	1401.77	K	Joback Method
tf	727.31	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.79	J/mol×K	1140.69	Joback Method
cpg	1453.66	J/mol×K	1184.20	Joback Method
cpg	1479.60	J/mol×K	1227.72	Joback Method
cpg	1505.88	J/mol×K	1271.23	Joback Method
cpg	1532.80	J/mol×K	1314.75	Joback Method
cpg	1560.63	J/mol×K	1358.26	Joback Method
cpg	1589.65	J/mol×K	1401.77	Joback Method

Sources

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=B6005428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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