5,6-dehydroisoandrosterone acetate

Inchi: InChI=1S/C21H30O3/c1-13(22)24-15-8-10-20(2)14(12-15)4-5-16-17-6-7-19(23)21(17,3)1
InchiKey: NCMZQTLCXHGLOK-UHFFFAOYSA-N
Formula: C21H30O3
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 330.47

Physical Properties

Property code	Value	Unit	Source
gf	-54.14	kJ/mol	Joback Method
hf	-562.76	kJ/mol	Joback Method
hfus	24.86	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-4.46		Aqueous Solubility Prediction Method
logp	4.450		Crippen Method
mcvol	268.020	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
tb	867.58	K	Joback Method
tc	1115.31	K	Joback Method
tf	573.57	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.49	J/mol×K	867.58	Joback Method
cpg	971.99	J/mol×K	908.87	Joback Method
cpg	998.46	J/mol×K	950.16	Joback Method
cpg	1025.25	J/mol×K	991.45	Joback Method
cpg	1052.70	J/mol×K	1032.74	Joback Method
cpg	1081.18	J/mol×K	1074.03	Joback Method
cpg	1111.01	J/mol×K	1115.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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