17-Ethylenedioxy-3alpha,5-cyclo-5alpha-androsta acetate

Inchi: InChI=1S/C23H34O4/c1-14(24)27-19-12-16-17(20(2)7-4-15-13-22(15,19)20)5-8-21(3)18
InchiKey: DDWOPNVMVRRBIH-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: CC(=O)OC1CC2C3CCC4(OCCO4)C3(C)CCC2C2(C)CCC3CC312
Mol. weight [g/mol]: 374.51
CAS: 1624-79-9

Physical Properties

Property code	Value	Unit	Source
gf	19.73	kJ/mol	Joback Method
hf	-608.59	kJ/mol	Joback Method
hfus	34.60	kJ/mol	Joback Method
hvap	79.43	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.314		Crippen Method
mcvol	288.950	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
tb	896.03	K	Joback Method
tc	1146.61	K	Joback Method
tf	654.23	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.30	J/mol×K	896.03	Joback Method
cpg	1126.90	J/mol×K	937.79	Joback Method
cpg	1165.40	J/mol×K	979.56	Joback Method
cpg	1207.59	J/mol×K	1021.32	Joback Method
cpg	1254.25	J/mol×K	1063.08	Joback Method
cpg	1306.18	J/mol×K	1104.84	Joback Method
cpg	1364.15	J/mol×K	1146.61	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=C1624799&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