3«alpha»-Propanoyloxy-5«alpha»-androstan-17-o

Other names: Etiocholan-3«alpha»-ol-17-one, propionate
Inchi: InChI=1S/C22H34O3/c1-4-20(24)25-15-9-11-21(2)14(13-15)5-6-16-17-7-8-19(23)22(17,3
InchiKey: SAOVUTZAPBDLOX-VYQAZBKGSA-N
Formula: C22H34O3
SMILES: CCC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CCC32)C1
Mol. weight [g/mol]: 346.50
CAS: 5953-68-4

Physical Properties

Property code	Value	Unit	Source
gf	-73.76	kJ/mol	Joback Method
hf	-650.05	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	75.25	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.920		Crippen Method
mcvol	286.410	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2400.00		NIST Webbook
tb	881.65	K	Joback Method
tc	1123.30	K	Joback Method
tf	567.32	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.52	J/mol×K	881.65	Joback Method
cpg	1069.44	J/mol×K	921.93	Joback Method
cpg	1097.22	J/mol×K	962.20	Joback Method
cpg	1125.19	J/mol×K	1002.48	Joback Method
cpg	1153.67	J/mol×K	1042.75	Joback Method
cpg	1182.99	J/mol×K	1083.03	Joback Method
cpg	1213.47	J/mol×K	1123.30	Joback Method

Sources

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=C5953684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume