

Androstan-17-ol, acetate, (5«alpha»,17«beta»)-

Other names:	5«alpha»-Androstan-17«beta»-ol, acetate 17«beta»-Acetoxy-5«alpha»-androstane 17«beta»-Hydroxy-5«alpha»-androstane acetate Androstan-17-yl acetate, (5«alpha»,17«beta»)- 17Beta-acetoxy-5alpha-androstane
Inchi:	InChI=1S/C21H34O2/c1-14(22)23-19-10-9-17-16-8-7-15-6-4-5-12-20(15,2)18(16)11-13-2
InchiKey:	QRRJQHVSHGOFL-LHOLKMYPKSA-N
Formula:	C21H34O2
SMILES:	CC(=O)OC1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]:	318.49
CAS:	1236-49-3

Physical Properties

Property code	Value	Unit	Source
gf	40.41	kJ/mol	Joback Method
hf	-491.71	kJ/mol	Joback Method
hfus	25.59	kJ/mol	Joback Method
hvap	68.78	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.351		Crippen Method
mcvol	270.750	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
tb	790.95	K	Joback Method
tc	1027.01	K	Joback Method
tf	487.83	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.29	J/mol×K	790.95	Joback Method
cpg	957.69	J/mol×K	830.29	Joback Method
cpg	984.44	J/mol×K	869.64	Joback Method
cpg	1010.88	J/mol×K	908.98	Joback Method

cpg	1037.35	J/mol×K	948.32	Joback Method
cpg	1064.19	J/mol×K	987.66	Joback Method
cpg	1091.75	J/mol×K	1027.01	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=C1236493&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

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