Ergostan-3-ol, acetate, (3«beta»,5«alpha»)-

Other names:	5«alpha»-Ergostan-3«beta»-ol, acetate
	Ergostan-3«beta»-yl acetate
	Ergostanol acetate
	Ergostanyl acetate
Inchi:	InChI=1S/C30H52O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31
InchiKey:	CVXQLNHSKSSFSQ-XMFXJLEFSA-N
Formula:	C30H52O2
SMILES:	CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)CCC(C)C(C)C)CCC32)C1
Mol. weight [g/mol]:	444.73
CAS:	4356-09-6

Physical Properties

Property code	Value	Unit	Source
gf	101.16	kJ/mol	Joback Method
hf	-713.65	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	8.285		Crippen Method
mcvol	397.560	ml/mol	McGowan Method
pc	852.47	kPa	Joback Method
rinpol	3287.00		NIST Webbook
tb	990.88	K	Joback Method
tc	1220.52	K	Joback Method
tf	540.02	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1537.25	J/mol×K	990.88	Joback Method
cpg	1571.26	J/mol×K	1029.15	Joback Method
cpg	1605.69	J/mol×K	1067.43	Joback Method
cpg	1640.87	J/mol×K	1105.70	Joback Method

cpg	1677.15	J/mol×K	1143.97	Joback Method
cpg	1714.87	J/mol×K	1182.25	Joback Method
cpg	1754.37	J/mol×K	1220.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4356096&Units=SI
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

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

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