

Stigmasta-7,22-dien-3-ol, acetate, (3«beta»,5«alpha»,22E)-

Other names:	5«alpha»-Stigmasta-7,22-dien-3«beta»-ol, acetate «alpha»-Spinasterol acetate «alpha»-Spinosterol acetate Spinasteryl acetate Spinasterol acetate
Inchi:	InChI=1S/C31H50O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5
InchiKey:	VQLULFBGTFJDEB-KPZAYUPNSA-N
Formula:	C31H50O2
SMILES:	CCC(C=CC(C)C1CCC2C3=CCC4CC(OC(C)=O)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]:	454.73
CAS:	4651-46-1

Physical Properties

Property code	Value	Unit	Source
gf	217.84	kJ/mol	Joback Method
hf	-550.42	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	90.79	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.372		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinpol	3353.00		NIST Webbook
tb	1026.73	K	Joback Method
tc	1263.18	K	Joback Method
tf	563.73	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1549.13	J/mol×K	1026.73	Joback Method
cpg	1584.84	J/mol×K	1066.14	Joback Method
cpg	1621.65	J/mol×K	1105.55	Joback Method

cpg	1659.95	J/mol×K	1144.96	Joback Method
cpg	1700.14	J/mol×K	1184.37	Joback Method
cpg	1742.62	J/mol×K	1223.77	Joback Method
cpg	1787.79	J/mol×K	1263.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4651461&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
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
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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