

5,24-Stigmastadienol 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:	IVUFTEWUONSFMP-ONGUEDQDSA-N
Formula:	C31H50O2
SMILES:	CCC(CCC(C)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C)=C(C)C
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	205.62	kJ/mol	Joback Method
hf	-559.44	kJ/mol	Joback Method
hfus	46.38	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.660		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	854.46	kPa	Joback Method
rinpol	3397.00		NIST Webbook
tb	1027.37	K	Joback Method
tc	1263.47	K	Joback Method
tf	565.81	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.25	J/molxK	1027.37	Joback Method
cpg	1584.19	J/molxK	1066.72	Joback Method
cpg	1621.28	J/molxK	1106.07	Joback Method
cpg	1659.92	J/molxK	1145.42	Joback Method
cpg	1700.51	J/molxK	1184.77	Joback Method
cpg	1743.43	J/molxK	1224.12	Joback Method
cpg	1789.10	J/molxK	1263.47	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=R110797&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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