

8(14)-Stigmastenol acetate, 24-«beta»

Other names:8(14)-Stigmastenol acetate, 24-«alpha»

Inchi:InChI=1S/C31H52O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5

InchiKey:OBDWLCLHGLNWSF-CTXIAVCRSA-N

Formula:C31H52O2

SMILES:CCC(CCC(C)C1CCC2=C3CCC4CC(OC(C)=O)CCC4(C)C3CCC21C)C(C)C

Mol. weight [g/mol]:456.74

Physical Properties

Property code	Value	Unit	Source
gf	135.70	kJ/mol	Joback Method
hf	-658.77	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	8.740		Crippen Method
mcvol	407.350	ml/mol	McGowan Method
pc	840.65	kPa	Joback Method
rinpol	3360.00		NIST Webbook
rinpol	3362.00		NIST Webbook
tb	1032.22	K	Joback Method
tc	1267.20	K	Joback Method
tf	585.57	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1575.08	J/mol×K	1032.22	Joback Method
cpg	1610.74	J/mol×K	1071.38	Joback Method
cpg	1647.40	J/mol×K	1110.55	Joback Method
cpg	1685.43	J/mol×K	1149.71	Joback Method
cpg	1725.20	J/mol×K	1188.87	Joback Method
cpg	1767.08	J/mol×K	1228.03	Joback Method
cpg	1811.45	J/mol×K	1267.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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