Fecosterol acetate

Inchi: InChI=1S/C30H48O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31)
InchiKey: QWRWBTVGCRGCNH-GROYKDTCSA-N
Formula: C30H48O2
SMILES: C=C(CCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(OC(C)=O)CC1CC3)C(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	209.01	kJ/mol	Joback Method
hf	-517.21	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	89.37	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.270		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
rinpol	3297.00		NIST Webbook
tb	1006.34	K	Joback Method
tc	1240.29	K	Joback Method
tf	573.58	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1470.76	J/mol×K	1006.34	Joback Method
cpg	1504.65	J/mol×K	1045.33	Joback Method
cpg	1539.45	J/mol×K	1084.32	Joback Method
cpg	1575.54	J/mol×K	1123.32	Joback Method
cpg	1613.28	J/mol×K	1162.31	Joback Method
cpg	1653.05	J/mol×K	1201.30	Joback Method
cpg	1695.22	J/mol×K	1240.29	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=R111205&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume