Ergosterol

Other names:	(22E)-ergosta-5,7,22-trien-3.beta.-ol
	(3«beta»)-Ergosta-5,7,22- trien-3-ol
	(3«beta»,22E)-Ergosta-5,7,22-trien-3-ol
	Ergosta-5,7,22-trien-3-ol, (3«beta»,22E)-
	Ergosterin
	Ergosterol, # 1
	Ergosterol, # 2
	Provitamin D
	Provitamin D2
Inchi:	InChI=1S/C28H44O/c1-18(2)19(3)7-8-20(4)24-11-12-25-23-10-9-21-17-22(29)13-15-27(2
InchiKey:	DNVPQKQSNYMLRS-CVGROQQCSA-N
Formula:	C28H44O
SMILES:	CC(C)C(C)C=CC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	396.65
CAS:	57-87-4

Physical Properties

Property code	Value	Unit	Source
chs	-16518.40	kJ/mol	NIST Webbook
gf	317.72	kJ/mol	Joback Method
hf	-329.28	kJ/mol	Joback Method
hfs	-788.20 ± 2.10	kJ/mol	NIST Webbook
hfus	35.25	kJ/mol	Joback Method
hsub	118.80	kJ/mol	NIST Webbook
hvap	92.89	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.331		Crippen Method
mcvol	354.910	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3152.00		NIST Webbook
rinpol	3080.00		NIST Webbook
rinpol	3144.00		NIST Webbook
rinpol	3123.00		NIST Webbook
rinpol	3087.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	982.79	K	Joback Method

tc	1211.92	K	Joback Method
tf	431.00	K	Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.55	J/mol×K	982.79	Joback Method
cpg	1358.23	J/mol×K	1020.98	Joback Method
cpg	1391.01	J/mol×K	1059.17	Joback Method
cpg	1425.25	J/mol×K	1097.35	Joback Method
cpg	1461.34	J/mol×K	1135.54	Joback Method
cpg	1499.64	J/mol×K	1173.73	Joback Method
cpg	1540.54	J/mol×K	1211.92	Joback Method
hsubt	147.00 ± 0.90	kJ/mol	365.00	NIST Webbook
hvapt	118.70	kJ/mol	437.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Sublimation Thermodynamic Parameters for Cholesterol, Ergosterol,:	https://www.doi.org/10.1021/je800395m
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=C57874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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