Lathosterol

Other names:	Cholest-7-en-3-ol, (3«beta»,5«alpha»)- 5«alpha»-Cholest-7-en-3«beta»-ol 3«beta»-Hydroxy-5«alpha»-cholest-7-ene 7-Cholesten-3-«beta»-ol Cholesterin «DELTA»7-Cholestenol Cholest-7-en-3-ol
Inchi:	InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4
InchiKey:	IZVFFXVYBHFIHY-VMTNTMNISA-N
Formula:	C27H46O
SMILES:	CC(C)CCCC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	386.65
CAS:	80-99-9

Physical Properties

Property code	Value	Unit	Source
gf	203.48	kJ/mol	Joback Method
hf	-487.23	kJ/mol	Joback Method
hfus	36.22	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.389		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	3170.00		NIST Webbook
tb	947.38	K	Joback Method
tc	1168.23	K	Joback Method
tf	527.39	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.89	J/mol×K	947.38	Joback Method

cpg	1347.08	J/mol×K	984.19	Joback Method
cpg	1377.74	J/mol×K	1021.00	Joback Method
cpg	1409.17	J/mol×K	1057.80	Joback Method
cpg	1441.71	J/mol×K	1094.61	Joback Method
cpg	1475.66	J/mol×K	1131.42	Joback Method
cpg	1511.34	J/mol×K	1168.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80999&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