Cholesta-8,24-dien-3-ol, (3«beta»,5«alpha»)-

Other names: 5«alpha»-Cholesta-8,24-dien-3«beta»-ol
Cholest-8,24-dien-3«beta»-ol
Zymosterol
Inchi: InChI=1S/C27H44O/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: CGSJXLIKVBJVRY-DLHVSSPOSA-N
Formula: C27H44O
SMILES: CC(C)=CCCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)CC1CC3
Mol. weight [g/mol]: 384.64
CAS: 128-33-6

Physical Properties

Property code	Value	Unit	Source
gf	275.67	kJ/mol	Joback Method
hf	-365.65	kJ/mol	Joback Method
hfus	37.17	kJ/mol	Joback Method
hvap	91.23	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.453		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
rinpol	3170.00		NIST Webbook
rinpol	3170.00		NIST Webbook
tb	961.51	K	Joback Method
tc	1187.24	K	Joback Method
tf	540.11	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.58	J/mol×K	961.51	Joback Method
cpg	1318.36	J/mol×K	999.13	Joback Method
cpg	1350.02	J/mol×K	1036.75	Joback Method
cpg	1382.90	J/mol×K	1074.38	Joback Method

cpg	1417.35	J/mol×K	1112.00	Joback Method
cpg	1453.74	J/mol×K	1149.62	Joback Method
cpg	1492.42	J/mol×K	1187.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C128336&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

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