Cholesta-5,7-dien-3-ol, (3«beta»)-

Other names:	Cholesta-5,7-dien-3«beta»-ol
	«DELTA»5,7-Cholesterol
	«DELTA»7-Cholesterol
	(3«beta»)-Cholesta-5,7-dien-3-ol
	Cholesterol, 7-dehydro-
	Dehydrocholesterol
	Provitamin D3
	5,7-Cholestandien-3«beta»-ol
	7-Dehydrocholesterin
	7-Dehydrocholesterol
	7,8-Didehydrocholesterol
	5,7-Cholestadien-3-«beta»-ol
	Dehydrocholesterin
	«DELTA»5,7-Cholestadien-3«beta»-ol
	NSC 18159
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:	UCTLRSWJYQTBFZ-CLVRJJFZSA-N
Formula:	C27H44O
SMILES:	CC(C)CCCC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	384.64
CAS:	434-16-2

Physical Properties

Property code	Value	Unit	Source
gf	231.52	kJ/mol	Joback Method
hf	-420.58	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	91.10	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.309		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	3160.00		NIST Webbook
rinpol	3160.00		NIST Webbook
tb	956.19	K	Joback Method
tc	1179.03	K	Joback Method
tf	544.91	K	Joback Method

vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.96	J/mol×K	956.19	Joback Method
cpg	1313.76	J/mol×K	993.33	Joback Method
cpg	1344.24	J/mol×K	1030.47	Joback Method
cpg	1375.73	J/mol×K	1067.61	Joback Method
cpg	1408.56	J/mol×K	1104.75	Joback Method
cpg	1443.06	J/mol×K	1141.89	Joback Method
cpg	1479.55	J/mol×K	1179.03	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C434162&Units=SI

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