Desmosterol

Other names:	24-Dehydrocholesterol
	Cholesta-5,24-dien-3-ol
	Cholesta-5,24-dien-3-ol, (3«beta»)-
	Cholesta-5,24-dien-3-ol, (3Â«betaÂ»)-
	Cholesta-5,24-dien-3«beta»-ol
	Cholesta-5,24-dien-3Â«betaÂ»-ol
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:	AVSXSVCZWQODGV-VUDDDUNTSA-N
Formula:	C27H44O
SMILES:	CC(C)=CCCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	384.64
CAS:	313-04-2

Physical Properties

Property code	Value	Unit	Source
gf	277.59	kJ/mol	Joback Method
hf	-374.52	kJ/mol	Joback Method
hfus	38.63	kJ/mol	Joback Method
hvap	90.26	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.309		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	3155.00		NIST Webbook
rinpol	3163.00		NIST Webbook
rinpol	3125.00		NIST Webbook
rinpol	3163.00		NIST Webbook
tb	951.86	K	Joback Method
tc	1176.29	K	Joback Method
tf	393.70	K	Solubility of Desmosterol in Five Organic Solvents
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.44	J/mol×K	951.86	Joback Method
cpg	1319.92	J/mol×K	989.27	Joback Method
cpg	1351.11	J/mol×K	1026.67	Joback Method
cpg	1383.35	J/mol×K	1064.08	Joback Method
cpg	1417.00	J/mol×K	1101.48	Joback Method
cpg	1452.39	J/mol×K	1138.89	Joback Method
cpg	1489.89	J/mol×K	1176.29	Joback Method
hfust	15.90	kJ/mol	388.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C313042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of cholesterol and desmosterol in binary solvent mixtures of n-hexane + ethanol:	https://www.doi.org/10.1016/j.fluid.2009.08.016
Solubility of Desmosterol in Five Organic Solvents:	https://www.doi.org/10.1021/je8006088
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
hfust:	Enthalpy of fusion at a given temperature
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