Cholecalciferol

Other names:	(3S,5Z,7E)-9,10-secocholesta-5,7,10-trien-3-ol (3«beta»,5Z,7E)-9,10-secocholesta-5,7,10(19)-trien-3-ol (S,Z)-3-(2-((1R,3aS,7aR,E)-7a-methyl-1-((R)-6-methylheptan-2-yl)octahydro-4H-inden-4-y 7-Dehydrocholesterol, activated 9,10-Secocholesta-5,7,10(19)-trien-3-ol, (3«beta»,5Z,7E)- 9,10-Secocholesta-5,7,10(19)-trien-3«beta»-ol Arachitol CC Calciol Cholecalciferol, D3 Colecalciferol Cyclohexanol, 3-[(2E)-2-[(1R,3aS,7aR)-1-[(1R)-1,5-dimethylhexyl]octahydro-7a-methyl-4H-inden-4-ylide D3-Vigantol (1S,3Z)- Delsterol Deparal Duphafral D3 1000 Ebivit Micro-dee NSC 375571 Oleovitamin D3 Provitina Quintox Ricketon Trivitan VidDe-3-hydrosol Vigantol Vigorsan Vitinc Dan-Dee-3 vitamin D3
Inchi:	InChI=1S/C27H44O/c1-19(2)8-6-9-21(4)25-15-16-26-22(10-7-17-27(25,26)5)12-13-23-18
InchiKey:	QYSXJUFSXHHAJI-SMGPGMQOSA-N
Formula:	C27H44O
SMILES:	C=C1CCC(O)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCCC(C)C
Mol. weight [g/mol]:	384.64
CAS:	67-97-0

Physical Properties

Property code	Value	Unit	Source
gf	275.21	kJ/mol	Joback Method
hf	-350.76	kJ/mol	Joback Method
hfus	38.79	kJ/mol	Joback Method
hvap	92.64	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.619		Crippen Method
mcvol	351.680	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
tb	962.31	K	Joback Method
tc	1183.65	K	Joback Method
tf	511.63	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1270.51	J/mol×K	962.31	Joback Method
cpg	1295.50	J/mol×K	999.20	Joback Method
cpg	1320.08	J/mol×K	1036.09	Joback Method
cpg	1344.47	J/mol×K	1072.98	Joback Method
cpg	1368.87	J/mol×K	1109.87	Joback Method
cpg	1393.48	J/mol×K	1146.76	Joback Method
cpg	1418.51	J/mol×K	1183.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Vitamin D3 in Six Organic Solvents at Temperatures from (248.2 to 273.2) K:	https://www.doi.org/10.1021/je300401c
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume