Ergocalciferol

Other names:

Vitamin D2
9,10-Secoergosta-5,7,10(19),22-tetraen-3-ol, (3«beta»,5Z,7E,22E)-
Buco-D
Calciferol
Condocaps
Condol
Crystallina
D-Arthin
Davitamon D
Davitin
Decaps
Dee-Osterol
Dee-Ron
Dee-Ronal
Deltalin
Deratol
Detalup
Diactol
Divit urto
Doral
Drisdol
Ergorone
Ertron
Fortodyl
Geltabs
Hi-Deratol
Infron
Metadee
Mulsiferol
Mykostin
Oleovitamin D2
Ostelin
Radiostol
Radsterin
Shock-ferol
Synthetic Vitamin D
Viosterol
Vitavel-D
Calciferon 2
Condacaps

Crtron
Daral
Dee-Roual
Ergosterol activated
Ergosterol, irradiated
Irradiated ergosta-5,7,22-trien-3«beta»-ol
Novovitamin-D
Oleovitamin D
Vigantol
Viostdrol
Vitamin D
9,10,Secoergosta-5,7,10(19),22-tetraen 3«beta»-ol
Sterogyl
Rodine C
(3«beta»,5Z,7E,22E)-9,10-Secoergosta-5,7,10(19)-,22-tetraen-3-ol
D-Tracetten
De-rat concentrate
Ercalciol
Uvesterol-D
Vio-D
(5Z,7E,22E)-9,10-Secoergosta-5,7,10,22-tetraen-3«beta»-ol
Cyclohexanol, 4-methylene-3-((2E)-2-((1R,3aS,7aR)-octahydro-7a-methyl-1-((1R,2E,4R)-1,4,5-trimethyl
(1) Vitamin D2
(1S,3Z)-
9,10-Secoergosta-5,7,10(19),22-tetraen-3.betat.-ol
Mina D2

Inchi: InChI=1S/C28H44O/c1-19(2)20(3)9-10-22(5)26-15-16-27-23(8-7-17-28(26,27)6)12-13-24

InchiKey: MECHNRXZTMCUDQ-HXLIECEWSA-N

Formula: C28H44O

SMILES: C=C1CCC(O)CC1=CC=C1CCCC2(C)C1CCC2C(C)C=CC(C)C(C)C

Mol. weight [g/mol]: 396.65

CAS: 50-14-6

Physical Properties

Property code	Value	Unit	Source
gf	361.41	kJ/mol	Joback Method
hf	-259.46	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	94.44	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method

logp	7.641		Crippen Method
mcvol	361.470	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
tb	988.91	K	Joback Method
tc	1216.45	K	Joback Method
tf	502.82	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1309.97	J/mol×K	988.91	Joback Method
cpg	1335.90	J/mol×K	1026.83	Joback Method
cpg	1361.69	J/mol×K	1064.76	Joback Method
cpg	1387.57	J/mol×K	1102.68	Joback Method
cpg	1413.79	J/mol×K	1140.60	Joback Method
cpg	1440.58	J/mol×K	1178.52	Joback Method
cpg	1468.20	J/mol×K	1216.45	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=C50146&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume