

17-(1,5-Dimethyl-hex-2-enyl)-10,13-dimethyl-2,3,4,

Other names:	Cholesta-5,7,22-trien-3-«beta»-ol 5,7,22-Cholestatrien-3«beta»-ol
Inchi:	InChI=1S/C27H42O/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:	RQOCXCFLRBRBCS-VURMDHGXSA-N
Formula:	C27H42O
SMILES:	CC(C)CC=CC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	382.62

Physical Properties

Property code	Value	Unit	Source
gf	311.74	kJ/mol	Joback Method
hf	-303.36	kJ/mol	Joback Method
hfus	36.18	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.085		Crippen Method
mcvol	340.820	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	3120.00		NIST Webbook
tb	960.35	K	Joback Method
tc	1187.04	K	Joback Method
tf	539.83	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.99	J/molxK	960.35	Joback Method
cpg	1287.08	J/molxK	998.13	Joback Method
cpg	1318.09	J/molxK	1035.91	Joback Method
cpg	1350.37	J/molxK	1073.70	Joback Method
cpg	1384.29	J/molxK	1111.48	Joback Method
cpg	1420.21	J/molxK	1149.26	Joback Method
cpg	1458.48	J/molxK	1187.04	Joback Method

Sources

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=U194794&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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