

Cholesta-5,22-dien-3-ol, (3«beta»)-

Other names:	Cholesta-5,22-dien-3«beta»-ol 22-Dehydrocholesterol 3«beta»-Cholesta-5,22-dien-3-ol Cholesta-5,22-dien-3-«beta»-ol, cis
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:	UPGTYLFCVNHBTN-QWKBDWIISA-N
Formula:	C27H44O
SMILES:	CC(C)CC=CC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	384.64
CAS:	92218-20-7

Physical Properties

Property code	Value	Unit	Source
gf	283.70	kJ/mol	Joback Method
hf	-370.01	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	89.79	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.165		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
tb	951.54	K	Joback Method
tc	1176.23	K	Joback Method
tf	522.31	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.10	J/molxK	951.54	Joback Method
cpg	1320.53	J/molxK	988.99	Joback Method
cpg	1351.64	J/molxK	1026.44	Joback Method
cpg	1383.79	J/molxK	1063.89	Joback Method
cpg	1417.31	J/molxK	1101.33	Joback Method

cpg	1452.57	J/mol×K	1138.78	Joback Method
cpg	1489.90	J/mol×K	1176.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92218207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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