Cholesta-5,25-dien-3-«beta»-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: RLFTZYOYELHUIM-VUDDDUNTSA-N
Formula: C27H44O
SMILES: C=C(C)CCCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 384.64

Physical Properties

Property code	Value	Unit	Source
gf	285.21	kJ/mol	Joback Method
hf	-366.31	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	89.63	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.309		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1106.68	kPa	Joback Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tb	944.38	K	Joback Method
tc	1166.26	K	Joback Method
tf	526.67	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.84	J/mol×K	944.38	Joback Method
cpg	1315.64	J/mol×K	981.36	Joback Method
cpg	1345.99	J/mol×K	1018.34	Joback Method
cpg	1377.21	J/mol×K	1055.32	Joback Method
cpg	1409.63	J/mol×K	1092.30	Joback Method
cpg	1443.57	J/mol×K	1129.28	Joback Method
cpg	1479.37	J/mol×K	1166.26	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=R215288&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume