Epicholestanol

Other names:	Cholestan-3-ol, (3«alpha»,5«alpha»)- 5«alpha»-Cholestan-3«alpha»-ol Cholestan-3«alpha»-ol Epidehydrocholesterin
Inchi:	InChI=1S/C27H48O/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:	QYIXCDOBOSTCEI-WXXXDBQUSA-N
Formula:	C27H48O
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	388.67
CAS:	516-95-0

Physical Properties

Property code	Value	Unit	Source
gf	175.44	kJ/mol	Joback Method
hf	-553.88	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.469		Crippen Method
mcvol	353.720	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinpol	3100.00		NIST Webbook
tb	938.57	K	Joback Method
tc	1157.43	K	Joback Method
tf	509.87	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1349.43	J/mol×K	938.57	Joback Method
cpg	1380.08	J/mol×K	975.05	Joback Method
cpg	1410.98	J/mol×K	1011.52	Joback Method
cpg	1442.45	J/mol×K	1048.00	Joback Method

cpg	1474.79	J/mol×K	1084.48	Joback Method
cpg	1508.30	J/mol×K	1120.95	Joback Method
cpg	1543.29	J/mol×K	1157.43	Joback Method

Sources

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=C516950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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