Cholestanol

Other names:	Cholestan-3-ol, (3«beta»,5«alpha»)- 5«alpha»-Cholestan-3«beta»-ol «beta»-Cholestanol Cholestan-3«beta»-ol Dihydrocholesterin Dihydrocholesterol Zymostanol 3«beta»-Hydroxy-5«alpha»-cholestane 3«beta»-Hydroxycholestane 5«alpha»-Cholestanol 5«alpha»-Dihydrocholesterol 3«beta»-Cholestanol NSC 18188
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-SWSAENCJSA-N
Formula:	C27H48O
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	388.67
CAS:	80-97-7

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	3115.00		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	1508.30	J/mol×K	1120.95	Joback Method
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	1543.29	J/mol×K	1157.43	Joback Method
hfust	22.60	kJ/mol	413.50	NIST Webbook

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=C80977&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
hfust: Enthalpy of fusion at a given temperature
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