Allocholesterol

Other names:	Cholest-4-en-3-ol, (3«beta»)-
	Cholest-4-en-3«beta»-ol
	Allocholesterin
	Coprostenol
	3«beta»-Hydroxycholest-4-ene
	4-Cholesten-3«beta»-ol
	4:5-Coprosten-3-ol
	(3«beta»)-Cholest-4-en-3-ol
Inchi:	InChI=1S/C27H46O/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:	UIMGHSAOLFTOBF-VUDDDUNTSA-N
Formula:	C27H46O
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4=CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	386.65
CAS:	517-10-2

Physical Properties

Property code	Value	Unit	Source
gf	203.48	kJ/mol	Joback Method
hf	-487.23	kJ/mol	Joback Method
hfus	36.22	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.389		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	947.38	K	Joback Method
tc	1168.23	K	Joback Method
tf	527.39	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.89	J/mol×K	947.38	Joback Method
cpg	1347.08	J/mol×K	984.19	Joback Method
cpg	1377.74	J/mol×K	1021.00	Joback Method
cpg	1409.17	J/mol×K	1057.80	Joback Method
cpg	1441.71	J/mol×K	1094.61	Joback Method
cpg	1475.66	J/mol×K	1131.42	Joback Method
cpg	1511.34	J/mol×K	1168.23	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=C517102&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

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