Cholesteryl methyl carbonate

Other names:	Carbonic acid, cholesteryl methyl ester
	Cholest-5-en-3-ol (3«beta»)-, methyl carbonate
	Cholesterol, methyl carbonate
	Cholest-5-en-3«beta»-yl-methyl carbonate
Inchi:	InChI=1S/C29H48O3/c1-19(2)8-7-9-20(3)24-12-13-25-23-11-10-21-18-22(32-27(30)31-6
InchiKey:	WHMGDIMLSAAHJQ-FOBBRWMUSA-N
Formula:	C29H48O3
SMILES:	COC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]:	444.69
CAS:	15507-52-5

Physical Properties

Property code	Value	Unit	Source
gf	18.22	kJ/mol	Joback Method
hf	-753.30	kJ/mol	Joback Method
hfus	41.28	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	8.179		Crippen Method
mcvol	385.040	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
tb	999.67	K	Joback Method
tc	1230.22	K	Joback Method
tf	583.50	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1470.42	J/mol×K	999.67	Joback Method
cpg	1503.00	J/mol×K	1038.10	Joback Method
cpg	1536.10	J/mol×K	1076.52	Joback Method
cpg	1570.05	J/mol×K	1114.95	Joback Method
cpg	1605.18	J/mol×K	1153.37	Joback Method

cpg	1641.82	J/mol×K	1191.80	Joback Method
cpg	1680.28	J/mol×K	1230.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15507525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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