Cholest-5-ene, 3-methoxy-, (3«beta»)-

Other names:	Cholest-5-ene, 3«beta»-methoxy-
	Cholesterin methyl ether
	Cholesterol methyl ether
	Cholesteryl methyl ether
	3«beta»-Methoxycholest-5-ene
	(3«beta»)-3-Methoxycholest-5-ene
	Cholest-5-en-3«beta»-yl-methyl ether
	3-Methoxycholest-5-ene, (3«beta»)-
	3-O-Methylcholesterol
	NSC 95435
Inchi:	InChI=1S/C28H48O/c1-19(2)8-7-9-20(3)24-12-13-25-23-11-10-21-18-22(29-6)14-16-27(2
InchiKey:	RCXPTZJNVLDKKV-UHFFFAOYSA-N
Formula:	C28H48O
SMILES:	COC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCCC(C)C)CCC32)C1
Mol. weight [g/mol]:	400.68
CAS:	1174-92-1

Physical Properties

Property code	Value	Unit	Source
chs	-17226.00 ± 5.00	kJ/mol	NIST Webbook
gf	243.72	kJ/mol	Joback Method
hf	-487.86	kJ/mol	Joback Method
hfs	-652.30 ± 5.40	kJ/mol	NIST Webbook
hfus	35.91	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	8.043		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	3216.80		NIST Webbook
tb	900.50	K	Joback Method
tc	1122.15	K	Joback Method
tf	500.07	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1328.02	J/mol×K	900.50	Joback Method
cpg	1359.07	J/mol×K	937.44	Joback Method
cpg	1390.03	J/mol×K	974.38	Joback Method
cpg	1421.18	J/mol×K	1011.32	Joback Method
cpg	1452.84	J/mol×K	1048.27	Joback Method
cpg	1485.31	J/mol×K	1085.21	Joback Method
cpg	1518.90	J/mol×K	1122.15	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1174921&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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