Methyl cholate

Other names:	Cholan-24-oic acid, 3,7,12-trihydroxy-, methyl ester, (3«alpha»,5«beta»,7«alpha»,12«alpha»)-
	Methyl 3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-cholanate
	Cholic acid, methyl ester
	Methyl 3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-cholanoate
	Methyl 3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-cholan-24-oate
	Cholanic (5«beta») acid, methyl ester
Inchi:	InChI=1S/C25H42O5/c1-14(5-8-22(29)30-4)17-6-7-18-23-19(13-21(28)25(17,18)3)24(2)1
InchiKey:	DLYVTEULDNMQAR-XQXZXKLNSA-N
Formula:	C25H42O5
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C
Mol. weight [g/mol]:	422.60
CAS:	1448-36-8

Physical Properties

Property code	Value	Unit	Source
gf	-361.94	kJ/mol	Joback Method
hf	-1097.26	kJ/mol	Joback Method
hfus	47.90	kJ/mol	Joback Method
hvap	126.40	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.537		Crippen Method
mcvol	344.720	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
ripol	3537.00		NIST Webbook
ripol	3537.00		NIST Webbook
tb	1144.56	K	Joback Method
tc	1412.67	K	Joback Method
tf	687.65	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.41	J/mol×K	1144.56	Joback Method
cpg	1514.54	J/mol×K	1189.24	Joback Method
cpg	1557.15	J/mol×K	1233.93	Joback Method
cpg	1602.74	J/mol×K	1278.61	Joback Method
cpg	1651.80	J/mol×K	1323.30	Joback Method
cpg	1704.82	J/mol×K	1367.98	Joback Method
cpg	1762.30	J/mol×K	1412.67	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=C1448368&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from:
https://www.chemeo.com/cid/71-849-1/Methyl-cholate.pdf