Cholan-24-oic acid, methyl ester, (5«beta»)-

Other names:	5«beta»-Cholan-24-oic acid, methyl ester
	Methyl cholanate
	Methyl 5«beta»-cholanate
	Methyl-5«beta»-cholan-24-oate
	Methyl-5«beta»-cholanoate
	5«beta»-Cholanic acid methyl ester
Inchi:	InChI=1S/C25H42O2/c1-17(8-13-23(26)27-4)20-11-12-21-19-10-9-18-7-5-6-15-24(18,2)2
InchiKey:	YHTRVWPOAJKWBV-UHFFFAOYSA-N
Formula:	C25H42O2
SMILES:	COC(=O)CCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]:	374.60
CAS:	2204-14-0

Physical Properties

Property code	Value	Unit	Source
gf	71.65	kJ/mol	Joback Method
hf	-579.55	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	77.30	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.625		Crippen Method
mcvol	327.110	ml/mol	McGowan Method
pc	1166.43	kPa	Joback Method
rinpol	2906.00		NIST Webbook
tb	882.03	K	Joback Method
tc	1109.48	K	Joback Method
tf	517.91	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.40	J/mol×K	882.03	Joback Method
cpg	1217.75	J/mol×K	919.94	Joback Method

cpg	1246.95	J/mol×K	957.85	Joback Method
cpg	1276.33	J/mol×K	995.76	Joback Method
cpg	1306.21	J/mol×K	1033.67	Joback Method
cpg	1336.90	J/mol×K	1071.58	Joback Method
cpg	1368.73	J/mol×K	1109.48	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=C2204140&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume