Cholan-24-oic acid, 3-(acetyloxy)-, methyl ester, (3«alpha»,5«beta»)-

Other names:	5«beta»-Cholanic acid, 3«alpha»-hydroxy-, methyl ester, acetate
	Acetyllithocholic acid, methyl ester
	Methyl lithocholate acetate
	Methyl 3«alpha»-acetoxylithocholate
	3«alpha»-Acetoxy-5«beta»-cholanic acid methyl ester
	5«beta»-Cholan-24-oic acid, 3«alpha»-hydroxy-, methyl ester, acetate
	Methyl 3-O-acetyllithocholate
	Lithocholic acid, acetate, methyl ester
Inchi:	InChI=1S/C27H44O4/c1-17(6-11-25(29)30-5)22-9-10-23-21-8-7-19-16-20(31-18(2)28)12
InchiKey:	DVIUCIPCTDVQAP-ACCPVXDNSA-N
Formula:	C27H44O4
SMILES:	COC(=O)CCC(C)C1CCC2C3CCC4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	432.64
CAS:	3253-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-153.14	kJ/mol	Joback Method
hf	-885.97	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	90.59	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.166		Crippen Method
mcvol	362.730	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3179.00		NIST Webbook
tb	999.41	K	Joback Method
tc	1232.41	K	Joback Method
tf	608.37	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1396.53	J/mol×K	999.41	Joback Method
cpg	1427.80	J/mol×K	1038.24	Joback Method
cpg	1459.57	J/mol×K	1077.08	Joback Method
cpg	1492.14	J/mol×K	1115.91	Joback Method
cpg	1525.84	J/mol×K	1154.74	Joback Method
cpg	1560.99	J/mol×K	1193.58	Joback Method
cpg	1597.92	J/mol×K	1232.41	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=C3253698&Units=SI

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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