Cholan-24-oic acid, 3-(acetyloxy)-7-oxo-, methyl ester, (3«alpha»,5«beta»)-

Inchi: InChI=1S/C27H42O5/c1-16(6-9-24(30)31-5)20-7-8-21-25-22(11-13-27(20,21)4)26(3)12-1

InchiKey: IOBLILNCUSICGD-AWWQQTNVSA-N

Formula: C27H42O5

SMILES: COC(=O)CCC(C)C1CCC2C3C(=O)CC4CC(OC(C)=O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 446.62

CAS: 10452-65-0

Physical Properties

Property code	Value	Unit	Source
gf	-275.73	kJ/mol	Joback Method
hf	-1023.67	kJ/mol	Joback Method
hfus	40.98	kJ/mol	Joback Method
hvap	94.84	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.345		Crippen Method
mcvol	364.300	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
tb	1067.23	K	Joback Method
tc	1312.03	K	Joback Method
tf	676.59	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1448.82	J/mol×K	1067.23	Joback Method
cpg	1481.24	J/mol×K	1108.03	Joback Method
cpg	1514.40	J/mol×K	1148.83	Joback Method
cpg	1548.63	J/mol×K	1189.63	Joback Method
cpg	1584.24	J/mol×K	1230.43	Joback Method
cpg	1621.57	J/mol×K	1271.23	Joback Method
cpg	1660.94	J/mol×K	1312.03	Joback Method

Sources

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=C10452650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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