

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

Other names:	Methyl 5-«beta»-cholan-3-one-24-oate
Inchi:	InChI=1S/C25H40O3/c1-16(5-10-23(27)28-4)20-8-9-21-19-7-6-17-15-18(26)11-13-24(17
InchiKey:	SRLWMUQGWKOYLX-UHFFFAOYSA-N
Formula:	C25H40O3
SMILES:	COC(=O)CCC(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	388.58
CAS:	1173-32-6

Physical Properties

Property code	Value	Unit	Source
gf	-50.94	kJ/mol	Joback Method
hf	-717.25	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	81.54	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.804		Crippen Method
mcvol	328.680	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	3124.00		NIST Webbook
tb	949.85	K	Joback Method
tc	1187.18	K	Joback Method
tf	586.13	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.66	J/molxK	949.85	Joback Method
cpg	1270.70	J/molxK	989.41	Joback Method
cpg	1300.95	J/molxK	1028.96	Joback Method
cpg	1331.71	J/molxK	1068.52	Joback Method
cpg	1363.32	J/molxK	1108.07	Joback Method
cpg	1396.09	J/molxK	1147.63	Joback Method
cpg	1430.34	J/molxK	1187.18	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=C1173326&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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