Chol-4-en-24-oic acid, 3-oxo-, methyl ester

Other names: 3-Oxochol-4-en-24-oic acid methyl ester
Methyl chol-4-en-3-one-24-oate
Inchi: InChI=1S/C25H38O3/c1-16(5-10-23(27)28-4)20-8-9-21-19-7-6-17-15-18(26)11-13-24(17
InchiKey: WDIPFMUQXPGENA-XPXBWSFBSA-N
Formula: C25H38O3
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 386.57
CAS: 1452-33-1

Physical Properties

Property code	Value	Unit	Source
gf	-22.90	kJ/mol	Joback Method
hf	-650.60	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.724		Crippen Method
mcvol	324.380	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	3233.00		NIST Webbook
rinpol	3233.00		NIST Webbook
tb	958.66	K	Joback Method
tc	1198.08	K	Joback Method
tf	603.65	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.16	J/mol×K	958.66	Joback Method
cpg	1236.70	J/mol×K	998.56	Joback Method
cpg	1266.67	J/mol×K	1038.47	Joback Method
cpg	1297.39	J/mol×K	1078.37	Joback Method
cpg	1329.21	J/mol×K	1118.27	Joback Method

cpg	1362.45	J/mol×K	1158.17	Joback Method
cpg	1397.46	J/mol×K	1198.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1452331&Units=SI
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

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