Cholest-4-en-3-one

Other names:	3-Oxocholest-4-ene
	Cholestenone
	«delta»4-Cholesten-3-one
	4-Cholestenone
	4-Cholesten-3-one
	(+)-4-Cholesten-3-one
Inchi:	InChI=1S/C27H44O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4
InchiKey:	NYOXRYYXRWJDKP-XUJZTTFYSA-N
Formula:	C27H44O
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	384.64
CAS:	601-57-0

Physical Properties

Property code	Value	Unit	Source
gf	225.42	kJ/mol	Joback Method
hf	-452.36	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	77.71	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.597		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	3245.00		NIST Webbook
tb	927.69	K	Joback Method
tc	1161.44	K	Joback Method
tf	539.03	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.88	J/mol×K	927.69	Joback Method
cpg	1307.11	J/mol×K	966.65	Joback Method

cpg	1338.52	J/mol×K	1005.61	Joback Method
cpg	1370.45	J/mol×K	1044.56	Joback Method
cpg	1403.26	J/mol×K	1083.52	Joback Method
cpg	1437.28	J/mol×K	1122.48	Joback Method
cpg	1472.84	J/mol×K	1161.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C601570&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

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