22-Ketocholest-3-one

Inchi: InChI=1S/C27H44O2/c1-17(2)6-11-25(29)18(3)22-9-10-23-21-8-7-19-16-20(28)12-14-26
InchiKey: REMYDTZFJKABEJ-SGPZLPSESA-N
Formula: C27H44O2
SMILES: CC(C)CCC(=O)C(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 400.64

Physical Properties

Property code	Value	Unit	Source
gf	68.46	kJ/mol	Joback Method
hf	-631.59	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.856		Crippen Method
mcvol	350.990	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	3380.00		NIST Webbook
rinpol	3380.00		NIST Webbook
tb	972.75	K	Joback Method
tc	1210.73	K	Joback Method
tf	571.44	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.98	J/mol×K	972.75	Joback Method
cpg	1374.06	J/mol×K	1012.41	Joback Method
cpg	1406.57	J/mol×K	1052.08	Joback Method
cpg	1439.87	J/mol×K	1091.74	Joback Method
cpg	1474.31	J/mol×K	1131.40	Joback Method
cpg	1510.24	J/mol×K	1171.06	Joback Method
cpg	1548.02	J/mol×K	1210.73	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=R528673&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