22-Ketocholesterol

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: ZJIBAMHOAQWYSE-UHFFFAOYSA-N
Formula: C27H44O2
SMILES: CC(C)CCC(=O)C(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 400.64

Physical Properties

Property code	Value	Unit	Source
gf	74.56	kJ/mol	Joback Method
hf	-599.81	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	96.58	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.568		Crippen Method
mcvol	350.990	ml/mol	McGowan Method
pc	1124.57	kPa	Joback Method
rinpol	3255.00		NIST Webbook
rinpol	3255.00		NIST Webbook
tb	1001.25	K	Joback Method
tc	1230.78	K	Joback Method
tf	577.32	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.21	J/mol×K	1001.25	Joback Method
cpg	1381.73	J/mol×K	1039.50	Joback Method
cpg	1414.24	J/mol×K	1077.76	Joback Method
cpg	1448.09	J/mol×K	1116.01	Joback Method
cpg	1483.64	J/mol×K	1154.27	Joback Method
cpg	1521.23	J/mol×K	1192.52	Joback Method
cpg	1561.21	J/mol×K	1230.78	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=U127063&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume