Cholesta-4,6-dien-3-one

Other names: 4,6-Cholestadien-3-one
4,6-Cholestadiene-3-one
Inchi: InChI=1S/C27H42O/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: XIWMRKFKSRYSIJ-XUJZTTFYSA-N
Formula: C27H42O
SMILES: CC(C)CCCC(C)C1CCC2C3C=CC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 382.62
CAS: 566-93-8

Physical Properties

Property code	Value	Unit	Source
gf	255.38	kJ/mol	Joback Method
hf	-394.58	kJ/mol	Joback Method
hfus	31.79	kJ/mol	Joback Method
hvap	78.01	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	7.373		Crippen Method
mcvol	340.820	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	3161.00		NIST Webbook
tb	926.85	K	Joback Method
tc	1161.81	K	Joback Method
tf	539.79	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1245.35	J/mol×K	926.85	Joback Method
cpg	1275.93	J/mol×K	966.01	Joback Method
cpg	1306.77	J/mol×K	1005.17	Joback Method
cpg	1338.22	J/mol×K	1044.33	Joback Method
cpg	1370.61	J/mol×K	1083.49	Joback Method
cpg	1404.31	J/mol×K	1122.65	Joback Method

cpg	1439.67	J/mol×K	1161.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C566938&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