

Cholesterol, 7-oxo-

Other names:	Cholest-5-en-7-one, 3-hydroxy-, (3«beta»)- Cholest-5-en-7-one, 3«beta»-hydroxy- 7-Ketocholesterol 7-Oxocholesterol SC 4722 3-Hydroxycholest-5-en-7-one-, (3«beta»)- 5-Cholesten-3«beta»-ol-7-one 3«beta»-Hydroxycholest-5-en-7-one
Inchi:	InChI=1S/C27H44O2/c1-17(2)7-6-8-18(3)21-9-10-22-25-23(12-14-27(21,22)5)26(4)13-11
InchiKey:	YIKKMWSQVKJCOP-SWTCZJJUSA-N
Formula:	C27H44O2
SMILES:	CC(C)CCCC(C)C1CCC2C3C(=O)C=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	400.64
CAS:	566-28-9

Physical Properties

Property code	Value	Unit	Source
gf	80.89	kJ/mol	Joback Method
hf	-624.93	kJ/mol	Joback Method
hfus	35.73	kJ/mol	Joback Method
hvap	94.08	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.568		Crippen Method
mcvol	350.990	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	3410.20		NIST Webbook
tb	1015.20	K	Joback Method
tc	1248.05	K	Joback Method
tf	595.61	K	Joback Method
vc	1.329	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	1371.68	J/mol×K	1015.20	Joback Method
cpg	1403.68	J/mol×K	1054.01	Joback Method
cpg	1436.52	J/mol×K	1092.82	Joback Method
cpg	1470.54	J/mol×K	1131.62	Joback Method
cpg	1506.06	J/mol×K	1170.43	Joback Method
cpg	1543.42	J/mol×K	1209.24	Joback Method
cpg	1582.95	J/mol×K	1248.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C566289&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

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