

Cholestan-6-one, (5«alpha»)-

Other names:	5«alpha»-Cholestan-6-one
Inchi:	InChI=1S/C27H46O/c1-18(2)9-8-10-19(3)21-12-13-22-20-17-25(28)24-11-6-7-15-26(24,4
InchiKey:	WSSZZUWWCXSGKJ-GZSNNDGRSA-N
Formula:	C27H46O
SMILES:	CC(C)CCCC(C)C1CCC2C3CC(=O)C4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]:	386.65
CAS:	570-46-7

Physical Properties

Property code	Value	Unit	Source
gf	197.38	kJ/mol	Joback Method
hf	-519.01	kJ/mol	Joback Method
hfus	30.81	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.677		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
tb	918.88	K	Joback Method
tc	1150.52	K	Joback Method
tf	521.51	K	Joback Method
vc	1.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.06	J/molxK	918.88	Joback Method
cpg	1339.92	J/molxK	957.49	Joback Method
cpg	1371.74	J/molxK	996.09	Joback Method
cpg	1403.86	J/molxK	1034.70	Joback Method
cpg	1436.61	J/molxK	1073.31	Joback Method
cpg	1470.31	J/molxK	1111.92	Joback Method
cpg	1505.29	J/molxK	1150.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C570467&Units=SI
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

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
hvp:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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