

6-Ketocholestanol

Other names:	Cholestan-6-one, 3-hydroxy-, (3«beta»,5«alpha»)- 5«alpha»-Cholestan-6-one, 3«beta»-hydroxy- 6-Oxocholestanol 3-Hydroxycholestan-6-one, (3«beta»,5«alpha»)-
Inchi:	InChI=1S/C27H46O2/c1-17(2)7-6-8-18(3)21-9-10-22-20-16-25(29)24-15-19(28)11-13-27
InchiKey:	JQMVKOQOLPGBBE-UHFFFAOYSA-N
Formula:	C27H46O2
SMILES:	<chem>CC(C)CCCC(C)C1CCC2C3CC(=O)C4CC(O)CCC4(C)C3CCC12C</chem>
Mol. weight [g/mol]:	402.65
CAS:	1175-06-0

Physical Properties

Property code	Value	Unit	Source
gf	52.85	kJ/mol	Joback Method
hf	-691.58	kJ/mol	Joback Method
hfus	35.97	kJ/mol	Joback Method
hvap	92.82	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.648		Crippen Method
mcvol	355.290	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	3340.00		NIST Webbook
rinpol	3340.00		NIST Webbook
tb	1006.39	K	Joback Method
tc	1237.27	K	Joback Method
tf	578.09	K	Joback Method
vc	1.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1405.61	J/mol×K	1006.39	Joback Method
cpg	1437.78	J/mol×K	1044.87	Joback Method
cpg	1470.57	J/mol×K	1083.35	Joback Method

cpg	1504.28	J/mol×K	1121.83	Joback Method
cpg	1539.25	J/mol×K	1160.31	Joback Method
cpg	1575.79	J/mol×K	1198.79	Joback Method
cpg	1614.22	J/mol×K	1237.27	Joback Method

Sources

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=C1175060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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