

6-Ketocholestan-3-one

Inchi:	InChI=1S/C27H44O2/c1-17(2)7-6-8-18(3)21-9-10-22-20-16-25(29)24-15-19(28)11-13-27
InchiKey:	LNGLEOIUQBVERRY-VZRDNAIESA-N
Formula:	C27H44O2
SMILES:	CC(C)CCCC(C)C1CCC2C3CC(=O)C4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	400.64

Physical Properties

Property code	Value	Unit	Source
gf	74.79	kJ/mol	Joback Method
hf	-656.71	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.856		Crippen Method
mvol	350.990	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	3345.00		NIST Webbook
rinpol	3345.00		NIST Webbook
tb	986.70	K	Joback Method
tc	1228.34	K	Joback Method
tf	589.73	K	Joback Method
vc	1.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1363.35	J/molxK	986.70	Joback Method
cpg	1395.93	J/molxK	1026.97	Joback Method
cpg	1428.78	J/molxK	1067.25	Joback Method
cpg	1462.22	J/molxK	1107.52	Joback Method
cpg	1496.60	J/molxK	1147.79	Joback Method
cpg	1532.24	J/molxK	1188.06	Joback Method
cpg	1569.48	J/molxK	1228.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R528935&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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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