2-Oxacholest-3-one

Inchi: InChI=1S/C26H44O2/c1-17(2)7-6-8-18(3)21-11-12-22-20-10-9-19-15-24(27)28-16-26(19
InchiKey: RCHXZNSUHOCQEX-WXRZGQSWSA-N
Formula: C26H44O2
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CC(=O)OCC4(C)C3CCC12C
Mol. weight [g/mol]: 388.63

Physical Properties

Property code	Value	Unit	Source
gf	102.84	kJ/mol	Joback Method
hf	-630.37	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	78.73	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.871		Crippen Method
mcvol	341.200	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	3235.00		NIST Webbook
tb	922.95	K	Joback Method
tc	1155.70	K	Joback Method
tf	536.81	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.20	J/mol×K	922.95	Joback Method
cpg	1312.25	J/mol×K	961.74	Joback Method
cpg	1343.33	J/mol×K	1000.53	Joback Method
cpg	1374.77	J/mol×K	1039.32	Joback Method
cpg	1406.89	J/mol×K	1078.12	Joback Method
cpg	1440.02	J/mol×K	1116.91	Joback Method
cpg	1474.49	J/mol×K	1155.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R528717&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