24-Methyl-5-«alpha»-cholesta-7,9(11),22-trien-3-«b

Inchi: InChI=1S/C28H44O/c1-18(2)19(3)7-8-20(4)24-11-12-25-23-10-9-21-17-22(29)13-15-27(2
InchiKey: XSMGJKKUFBTARU-HOKDKEKWSA-N
Formula: C28H44O
SMILES: CC(C)C(C)C=CC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3=CCC21C
Mol. weight [g/mol]: 396.65

Physical Properties

Property code	Value	Unit	Source
gf	317.72	kJ/mol	Joback Method
hf	-329.28	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	92.89	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.331		Crippen Method
mcvol	354.910	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	3185.00		NIST Webbook
rinpol	3185.00		NIST Webbook
tb	982.79	K	Joback Method
tc	1211.92	K	Joback Method
tf	536.10	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.55	J/mol×K	982.79	Joback Method
cpg	1358.23	J/mol×K	1020.98	Joback Method
cpg	1391.01	J/mol×K	1059.17	Joback Method
cpg	1425.25	J/mol×K	1097.35	Joback Method
cpg	1461.34	J/mol×K	1135.54	Joback Method
cpg	1499.64	J/mol×K	1173.73	Joback Method
cpg	1540.54	J/mol×K	1211.92	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=R214834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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