24-Methyl-5-«alpha»-cholesta-8(14),22-dien-3-«be

Inchi: InChI=1S/C28H46O/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: ODJPLGNAFXMITB-ZAANIKMKSA-N
Formula: C28H46O
SMILES: CC(C)C(C)C=CC(C)C1CCC2=C3CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 398.66

Physical Properties

Property code	Value	Unit	Source
gf	287.76	kJ/mol	Joback Method
hf	-387.06	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	92.60	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.555		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	3160.00		NIST Webbook
rinpol	3160.00		NIST Webbook
tb	983.63	K	Joback Method
tc	1212.15	K	Joback Method
tf	535.34	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1358.24	J/mol×K	983.63	Joback Method
cpg	1390.54	J/mol×K	1021.72	Joback Method
cpg	1423.85	J/mol×K	1059.80	Joback Method
cpg	1458.56	J/mol×K	1097.89	Joback Method
cpg	1495.02	J/mol×K	1135.97	Joback Method
cpg	1533.62	J/mol×K	1174.06	Joback Method
cpg	1574.73	J/mol×K	1212.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490489&Units=SI

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