24-Methyl-5-«alpha»-cholest-14-en-3-«beta»-ol

Inchi: InChI=1S/C28H48O/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: TZMNZSROTXXMLX-MCEMEMKGSA-N
Formula: C28H48O
SMILES: CC(C)C(C)CCC(C)C1CC=C2C3CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 400.68

Physical Properties

Property code	Value	Unit	Source
gf	209.46	kJ/mol	Joback Method
hf	-513.15	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	91.67	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.635		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	1018.78	kPa	Joback Method
rinpol	3215.00		NIST Webbook
tb	969.82	K	Joback Method
tc	1193.49	K	Joback Method
tf	523.66	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1386.76	J/mol×K	969.82	Joback Method
cpg	1418.35	J/mol×K	1007.10	Joback Method
cpg	1450.56	J/mol×K	1044.38	Joback Method
cpg	1483.71	J/mol×K	1081.65	Joback Method
cpg	1518.15	J/mol×K	1118.93	Joback Method
cpg	1554.19	J/mol×K	1156.21	Joback Method
cpg	1592.18	J/mol×K	1193.49	Joback Method

Sources

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=R214730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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