24-Methylcholesta-5,24-dien-3-«beta»-ol

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: YTFTXKBJICNYCV-ZFLYDEBFSA-N
Formula: C28H46O
SMILES: CC(C)=C(C)CCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 398.66

Physical Properties

Property code	Value	Unit	Source
gf	277.46	kJ/mol	Joback Method
hf	-404.95	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.699		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	3270.00		NIST Webbook
rinpol	3270.00		NIST Webbook
tb	974.62	K	Joback Method
tc	1201.33	K	Joback Method
tf	520.66	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1358.65	J/mol×K	974.62	Joback Method
cpg	1390.71	J/mol×K	1012.40	Joback Method
cpg	1423.65	J/mol×K	1050.19	Joback Method
cpg	1457.86	J/mol×K	1087.97	Joback Method
cpg	1493.69	J/mol×K	1125.76	Joback Method
cpg	1531.51	J/mol×K	1163.54	Joback Method
cpg	1571.68	J/mol×K	1201.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490503&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

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