4-«alpha»,24-Dimethylcholest-8-en-3-«beta»-ol

Inchi: InChI=1S/C29H50O/c1-18(2)19(3)8-9-20(4)23-12-13-25-22-10-11-24-21(5)27(30)15-17-2
InchiKey: KLLFGBWPBOBVAC-OSRLTYJOSA-N
Formula: C29H50O
SMILES: CC(C)C(C)CCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)C(C)C1CC3
Mol. weight [g/mol]: 414.71

Physical Properties

Property code	Value	Unit	Source
gf	208.25	kJ/mol	Joback Method
hf	-545.26	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	94.56	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	8.025		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	3295.00		NIST Webbook
rinpol	3295.00		NIST Webbook
tb	997.68	K	Joback Method
tc	1224.44	K	Joback Method
tf	547.45	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.83	J/mol×K	997.68	Joback Method
cpg	1492.08	J/mol×K	1035.47	Joback Method
cpg	1526.16	J/mol×K	1073.27	Joback Method
cpg	1561.38	J/mol×K	1111.06	Joback Method
cpg	1598.10	J/mol×K	1148.85	Joback Method
cpg	1636.66	J/mol×K	1186.64	Joback Method
cpg	1677.41	J/mol×K	1224.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214998&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