

4-«alpha»,24-Dimethylcholest-8,14-dien-3-«beta»-

Inchi:	InChI=1S/C29H48O/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:	YKDJEAIZFMBVFZ-CYHCYTOHSA-N
Formula:	C29H48O
SMILES:	CC(C)C(C)CCC(C)C1CC=C2C3=C(CCC21C)C1(C)CCC(O)C(C)C1CC3
Mol. weight [g/mol]:	412.69

Physical Properties

Property code	Value	Unit	Source
gf	236.29	kJ/mol	Joback Method
hf	-478.61	kJ/mol	Joback Method
hfus	37.25	kJ/mol	Joback Method
hvap	95.83	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.945		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	982.69	kPa	Joback Method
rinpol	3280.00		NIST Webbook
tb	1006.49	K	Joback Method
tc	1235.21	K	Joback Method
tf	564.97	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1425.41	J/molxK	1006.49	Joback Method
cpg	1458.54	J/molxK	1044.61	Joback Method
cpg	1492.71	J/molxK	1082.73	Joback Method
cpg	1528.29	J/molxK	1120.85	Joback Method
cpg	1565.62	J/molxK	1158.97	Joback Method
cpg	1605.07	J/molxK	1197.09	Joback Method
cpg	1646.97	J/molxK	1235.21	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=R214978&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
mccvol:	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

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