

4-«alpha»,24-Dimethylcholest-8,24(28)-dien-3-«be

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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

QLDNWJOJCDIMKK-JWPWOQFDSA-N

C29H48O

C=C(CCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)C(C)C1CC3)C(C)C

412.69

Physical Properties

Property code	Value	Unit	Source
gf	289.98	kJ/mol	Joback Method
hf	-424.34	kJ/mol	Joback Method
hfus	38.42	kJ/mol	Joback Method
hvap	94.36	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.945		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	973.52	kPa	Joback Method
rinpol	3305.00		NIST Webbook
tb	994.68	K	Joback Method
tc	1221.84	K	Joback Method
tf	546.73	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1426.95	J/mol×K	994.68	Joback Method
cpg	1459.84	J/mol×K	1032.54	Joback Method
cpg	1493.64	J/mol×K	1070.40	Joback Method
cpg	1528.69	J/mol×K	1108.26	Joback Method
cpg	1565.33	J/mol×K	1146.12	Joback Method
cpg	1603.93	J/mol×K	1183.98	Joback Method
cpg	1644.83	J/mol×K	1221.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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