24-Methyl-5-«alpha»-cholesta-8,24(28)-dien-3-«be

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: SLQKYSPHBZMASJ-MXRIHRFBSA-N
Formula: C28H46O
SMILES: C=C(CCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)CC1CC3)C(C)C
Mol. weight [g/mol]: 398.66

Physical Properties

Property code	Value	Unit	Source
gf	289.27	kJ/mol	Joback Method
hf	-383.36	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	92.44	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.699		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1056.88	kPa	Joback Method
rinpol	3230.00		NIST Webbook
tb	976.47	K	Joback Method
tc	1202.38	K	Joback Method
tf	539.70	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.63	J/mol×K	976.47	Joback Method
cpg	1385.21	J/mol×K	1014.12	Joback Method
cpg	1417.64	J/mol×K	1051.77	Joback Method
cpg	1451.28	J/mol×K	1089.43	Joback Method
cpg	1486.49	J/mol×K	1127.08	Joback Method
cpg	1523.60	J/mol×K	1164.73	Joback Method
cpg	1562.97	J/mol×K	1202.38	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=R214869&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