4-«beta»-Methylcholest-5-en-3-«beta»-ol

Inchi: InChI=1S/C28H48O/c1-18(2)8-7-9-19(3)22-12-13-24-21-10-11-23-20(4)26(29)15-17-28(2
InchiKey: PZELUKPNJYWGOY-PAZSGVRGSA-N
Formula: C28H48O
SMILES: CC(C)CCCC(C)C1CCC2C3CC=C4C(C)C(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 400.68

Physical Properties

Property code	Value	Unit	Source
gf	204.19	kJ/mol	Joback Method
hf	-528.21	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	91.75	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.635		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
rinpol	3150.00		NIST Webbook
tb	965.59	K	Joback Method
tc	1187.42	K	Joback Method
tf	534.42	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1389.24	J/mol×K	965.59	Joback Method
cpg	1420.61	J/mol×K	1002.56	Joback Method
cpg	1452.48	J/mol×K	1039.53	Joback Method
cpg	1485.16	J/mol×K	1076.51	Joback Method
cpg	1518.98	J/mol×K	1113.48	Joback Method
cpg	1554.23	J/mol×K	1150.45	Joback Method
cpg	1591.25	J/mol×K	1187.42	Joback Method

Sources

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=R215060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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