4,4,14-«alpha»-Trimethyl-5-«alpha»-cholest-8-en-3

Inchi: InChI=1S/C30H52O/c1-20(2)10-9-11-21(3)22-14-18-30(8)24-12-13-25-27(4,5)26(31)16-1
InchiKey: MBZYKEVPFYHDOH-BZBIHAHBSA-N
Formula: C30H52O
SMILES: CC(C)CCCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(O)C(C)(C)C1CC3
Mol. weight [g/mol]: 428.73

Physical Properties

Property code	Value	Unit	Source
gf	208.13	kJ/mol	Joback Method
hf	-530.14	kJ/mol	Joback Method
hfus	31.00	kJ/mol	Joback Method
hvap	94.87	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.559		Crippen Method
mcvol	391.690	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	3265.00		NIST Webbook
rinpol	3265.00		NIST Webbook
tb	1021.48	K	Joback Method
tc	1253.56	K	Joback Method
tf	621.52	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1551.44	J/mol×K	1021.48	Joback Method
cpg	1598.60	J/mol×K	1060.16	Joback Method
cpg	1649.29	J/mol×K	1098.84	Joback Method
cpg	1704.10	J/mol×K	1137.52	Joback Method
cpg	1763.60	J/mol×K	1176.20	Joback Method
cpg	1828.37	J/mol×K	1214.88	Joback Method
cpg	1898.99	J/mol×K	1253.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490518&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

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