4,4,14-«alpha»-Trimethyl-5-«alpha»-cholest-7-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: BTWVJMHYCKBVBM-UAQMTODXSA-N
Formula: C30H52O
SMILES: CC(C)CCCC(C)C1CCC2(C)C3=CCC4C(C)(C)C(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 428.73

Physical Properties

Property code	Value	Unit	Source
gf	210.05	kJ/mol	Joback Method
hf	-539.01	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	93.90	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	8.415		Crippen Method
mcvol	391.690	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	3305.00		NIST Webbook
tb	1011.83	K	Joback Method
tc	1242.27	K	Joback Method
tf	604.76	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1549.85	J/mol×K	1011.83	Joback Method
cpg	1595.82	J/mol×K	1050.24	Joback Method
cpg	1645.07	J/mol×K	1088.64	Joback Method
cpg	1698.15	J/mol×K	1127.05	Joback Method
cpg	1755.63	J/mol×K	1165.46	Joback Method
cpg	1818.09	J/mol×K	1203.86	Joback Method
cpg	1886.07	J/mol×K	1242.27	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=R214918&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
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