4,14-dimethyl,24-ethyl-cholestane

Inchi: InChI=1S/C31H56/c1-9-24(21(2)3)13-12-23(5)26-16-19-31(8)28-15-14-25-22(4)11-10-18
InchiKey: BNLOBOUNNLHEFC-DTOAWKGKSA-N
Formula: C31H56
SMILES: CCC(CCC(C)C1CCC2(C)C3CCC4C(C)CCCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 428.78

Physical Properties

Property code	Value	Unit	Source
gf	338.01	kJ/mol	Joback Method
hf	-474.25	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	79.26	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	9.770		Crippen Method
mcvol	404.210	ml/mol	McGowan Method
pc	806.16	kPa	Joback Method
rinpol	3232.00		NIST Webbook
tb	937.71	K	Joback Method
tc	1162.31	K	Joback Method
tf	503.03	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1532.59	J/mol×K	937.71	Joback Method
cpg	1570.82	J/mol×K	975.14	Joback Method
cpg	1610.05	J/mol×K	1012.58	Joback Method
cpg	1650.70	J/mol×K	1050.01	Joback Method
cpg	1693.23	J/mol×K	1087.44	Joback Method
cpg	1738.05	J/mol×K	1124.87	Joback Method
cpg	1785.61	J/mol×K	1162.31	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=R406018&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