cholestane

Other names: [8R-[8«alpha»,9«beta»,10«alpha»,13«alpha»,14«beta»,17«alpha»(R)]]-17-(1,5-dimethylh
Inchi: InChI=1S/C27H48/c1-19(2)9-8-10-20(3)23-14-15-24-22-13-12-21-11-6-7-17-26(21,4)25(2
InchiKey: XIIAYQZJNBULGD-UJBDRAHFSA-N
Formula: C27H48
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]: 372.67
CAS: 14982-53-7

Physical Properties

Property code	Value	Unit	Source
gf	319.97	kJ/mol	Joback Method
hf	-381.31	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	8.498		Crippen Method
mcvol	347.850	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
tb	851.06	K	Joback Method
tc	1072.72	K	Joback Method
tf	353.00 ± 4.00	K	NIST Webbook
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.75	J/mol×K	851.06	Joback Method
cpg	1282.08	J/mol×K	888.00	Joback Method
cpg	1312.99	J/mol×K	924.95	Joback Method
cpg	1343.81	J/mol×K	961.89	Joback Method
cpg	1374.86	J/mol×K	998.83	Joback Method
cpg	1406.45	J/mol×K	1035.78	Joback Method
cpg	1438.92	J/mol×K	1072.72	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=C14982537&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume