Cholest-4-ene

Inchi: InChI=1S/C27H46/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: YWHWYTRNKBGSRE-OYZXCHQLSA-N
Formula: C27H46
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4=CCCCC4(C)C3CCC12C
Mol. weight [g/mol]: 370.65
CAS: 16732-86-8

Physical Properties

Property code	Value	Unit	Source
gf	348.01	kJ/mol	Joback Method
hf	-314.66	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	73.47	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	8.418		Crippen Method
mcvol	343.550	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
tb	859.87	K	Joback Method
tc	1083.70	K	Joback Method
tf	355.00 ± 5.00	K	NIST Webbook
tf	351.00 ± 5.00	K	NIST Webbook
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.67	J/mol×K	859.87	Joback Method
cpg	1251.10	J/mol×K	897.17	Joback Method
cpg	1281.31	J/mol×K	934.48	Joback Method
cpg	1311.63	J/mol×K	971.78	Joback Method
cpg	1342.40	J/mol×K	1009.09	Joback Method
cpg	1373.96	J/mol×K	1046.39	Joback Method
cpg	1406.63	J/mol×K	1083.70	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=C16732868&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