

Cholest-3-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:	SFBMPHLOQAKIBY-UHFFFAOYSA-N
Formula:	C27H46
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4C=CCCC4(C)C3CCC12C
Mol. weight [g/mol]:	370.65
CAS:	16732-84-6

Physical Properties

Property code	Value	Unit	Source
gf	349.93	kJ/mol	Joback Method
hf	-323.53	kJ/mol	Joback Method
hfus	32.52	kJ/mol	Joback Method
hvap	72.50	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	8.274		Crippen Method
mcvol	343.550	ml/mol	McGowan Method
pc	1025.97	kPa	Joback Method
tb	850.22	K	Joback Method
tc	1073.17	K	Joback Method
tf	347.20 ± 2.00	K	NIST Webbook
vc	1.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.97	J/mol×K	850.22	Joback Method
cpg	1252.59	J/mol×K	887.38	Joback Method
cpg	1282.85	J/mol×K	924.54	Joback Method
cpg	1313.07	J/mol×K	961.69	Joback Method
cpg	1343.59	J/mol×K	998.85	Joback Method
cpg	1374.74	J/mol×K	1036.01	Joback Method
cpg	1406.84	J/mol×K	1073.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16732846&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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