Cholesta-3,5-diene

Other names:	«delta»(3,5)-Cholestadiene
	Cholesterilene
	Cholestadiene
	3,5-Cholestadiene
	Cholest-3,5-diene
	D3,5-cholestadiene
Inchi:	InChI=1S/C27H44/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:	RLHIRZFWJBOHHD-UHFFFAOYSA-N
Formula:	C27H44
SMILES:	CC(C)CCCC(C)C1CCC2C3CC=C4C=CCCC4(C)C3CCC12C
Mol. weight [g/mol]:	368.64
CAS:	747-90-0

Physical Properties

Property code	Value	Unit	Source
gf	377.97	kJ/mol	Joback Method
hf	-256.88	kJ/mol	Joback Method
hfus	32.28	kJ/mol	Joback Method
hvap	73.76	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	8.194		Crippen Method
mcvol	339.250	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	2880.00		NIST Webbook
rinpol	2880.00		NIST Webbook
tb	859.03	K	Joback Method
tc	1084.16	K	Joback Method
tf	471.57	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.70	J/mol×K	859.03	Joback Method

cpg	1221.42	J/mol×K	896.55	Joback Method
cpg	1250.97	J/mol×K	934.07	Joback Method
cpg	1280.70	J/mol×K	971.60	Joback Method
cpg	1310.96	J/mol×K	1009.12	Joback Method
cpg	1342.08	J/mol×K	1046.64	Joback Method
cpg	1374.41	J/mol×K	1084.16	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=C747900&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