

Cholest-5-ene, 3«beta»-chloro-

Other names:

Cholesteryl chloride
Cholest-5-ene, 3-chloro-, (3«beta»)-
Cholesterol chloride
3«beta»-Chlorocholest-5-ene
3-Chlorocholestene
5-Cholesten-3«beta»-chloride
3-Chlorocholest-5-ene-, (3«beta»)-
Cholest-5-ene, 3beta-chloro

Inchi:

InChI=1S/C27H45Cl/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,

InchiKey:

OTVRYZXVVMZHHW-HFRBDLMJSA-N

Formula:

C27H45Cl

SMILES:

CC(C)CCCC(C)C1CCC2C3CC=C4CC(Cl)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

405.10

CAS:

910-31-6

Physical Properties

Property code	Value	Unit	Source
gf	328.37	kJ/mol	Joback Method
hf	-350.74	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	77.54	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.635		Crippen Method
mcvol	355.790	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	892.63	K	Joback Method
tc	1119.74	K	Joback Method
tf	496.49	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.88	J/mol×K	892.63	Joback Method
cpg	1293.40	J/mol×K	930.48	Joback Method
cpg	1323.95	J/mol×K	968.33	Joback Method
cpg	1354.86	J/mol×K	1006.18	Joback Method
cpg	1386.49	J/mol×K	1044.03	Joback Method
cpg	1419.18	J/mol×K	1081.89	Joback Method
cpg	1453.27	J/mol×K	1119.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C910316&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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