3-chloro-24-methyl-«delta»5-Cholestene

Inchi: InChI=1S/C28H47Cl/c1-18(2)19(3)7-8-20(4)24-11-12-25-23-10-9-21-17-22(29)13-15-27(
InchiKey: BROSQZDTRZJAHJ-QTGZJRLASA-N
Formula: C28H47Cl
SMILES: CC(C)C(C)CCC(C)C1CCC2C3CC=C4CC(Cl)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 419.13

Physical Properties

Property code	Value	Unit	Source
gf	334.35	kJ/mol	Joback Method
hf	-376.66	kJ/mol	Joback Method
hfus	35.39	kJ/mol	Joback Method
hvap	79.38	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	8.881		Crippen Method
mcvol	369.880	ml/mol	McGowan Method
pc	939.79	kPa	Joback Method
rinpol	3170.00		NIST Webbook
tb	915.07	K	Joback Method
tc	1143.42	K	Joback Method
tf	492.76	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.26	J/mol×K	915.07	Joback Method
cpg	1362.80	J/mol×K	953.13	Joback Method
cpg	1394.50	J/mol×K	991.19	Joback Method
cpg	1426.72	J/mol×K	1029.24	Joback Method
cpg	1459.81	J/mol×K	1067.30	Joback Method
cpg	1494.12	J/mol×K	1105.36	Joback Method
cpg	1530.00	J/mol×K	1143.42	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=R163003&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