3-chloro-24-ethyl-«delta»5,22-Cholestadiene

Inchi: InChI=1S/C29H47Cl/c1-7-21(19(2)3)9-8-20(4)25-12-13-26-24-11-10-22-18-23(30)14-16-
InchiKey: CWRKLTLDSODKIL-CMDGGOBGSA-N
Formula: C29H47Cl
SMILES: CCC(C=CC(C)C1CCC2C3CC=C4CC(Cl)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 431.14

Physical Properties

Property code	Value	Unit	Source
gf	422.99	kJ/mol	Joback Method
hf	-280.08	kJ/mol	Joback Method
hfus	38.19	kJ/mol	Joback Method
hvap	81.56	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	9.047		Crippen Method
mcvol	379.670	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
tb	942.11	K	Joback Method
tc	1174.67	K	Joback Method
tf	498.95	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1373.84	J/mol×K	942.11	Joback Method
cpg	1406.58	J/mol×K	980.87	Joback Method
cpg	1439.86	J/mol×K	1019.63	Joback Method
cpg	1474.08	J/mol×K	1058.39	Joback Method
cpg	1509.64	J/mol×K	1097.15	Joback Method
cpg	1546.92	J/mol×K	1135.91	Joback Method
cpg	1586.32	J/mol×K	1174.67	Joback Method

Sources

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=R162986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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