24-methyl-«delta»3,5-Cholestadiene

Inchi: InChI=1S/C28H46/c1-19(2)20(3)10-11-21(4)24-14-15-25-23-13-12-22-9-7-8-17-27(22,5)2
InchiKey: TZFSYLGHXUOJOH-GSSRKXLNSA-N
Formula: C28H46
SMILES: CC(C)C(C)CCC(C)C1CCC2C3CC=C4C=CCCC4(C)C3CCC12C
Mol. weight [g/mol]: 382.66

Physical Properties

Property code	Value	Unit	Source
gf	383.95	kJ/mol	Joback Method
hf	-282.80	kJ/mol	Joback Method
hfus	31.35	kJ/mol	Joback Method
hvap	75.60	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	8.440		Crippen Method
mcvol	353.340	ml/mol	McGowan Method
pc	1003.98	kPa	Joback Method
rinpol	2950.00		NIST Webbook
tb	881.47	K	Joback Method
tc	1107.60	K	Joback Method
tf	467.84	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.93	J/mol×K	881.47	Joback Method
cpg	1289.58	J/mol×K	919.16	Joback Method
cpg	1320.20	J/mol×K	956.85	Joback Method
cpg	1351.14	J/mol×K	994.53	Joback Method
cpg	1382.75	J/mol×K	1032.22	Joback Method
cpg	1415.38	J/mol×K	1069.91	Joback Method
cpg	1449.39	J/mol×K	1107.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R162966&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

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