24-Ethyl-5-«alpha»-cholest-14,22-dien-3-«beta»-ol

Inchi: InChI=1S/C29H48O/c1-7-21(19(2)3)9-8-20(4)25-12-13-26-24-11-10-22-18-23(30)14-16-2
InchiKey: QALFHONQGOBQAA-AFHZOUOASA-N
Formula: C29H48O
SMILES: CCC(C=CC(C)C1CC=C2C3CCC4CC(O)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]: 412.69

Physical Properties

Property code	Value	Unit	Source
gf	298.10	kJ/mol	Joback Method
hf	-416.57	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	93.86	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	7.801		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	990.75	kPa	Joback Method
rinpol	3255.00		NIST Webbook
tb	996.86	K	Joback Method
tc	1225.48	K	Joback Method
tf	529.85	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1430.59	J/mol×K	996.86	Joback Method
cpg	1463.99	J/mol×K	1034.96	Joback Method
cpg	1498.43	J/mol×K	1073.07	Joback Method
cpg	1534.27	J/mol×K	1111.17	Joback Method
cpg	1571.91	J/mol×K	1149.28	Joback Method
cpg	1611.70	J/mol×K	1187.38	Joback Method
cpg	1654.02	J/mol×K	1225.48	Joback Method

Sources

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=R214547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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