24-Ethylcholesta-8,14,24(28)-trien-3-«beta»-ol

Inchi: InChI=1S/C29H46O/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: MZYZVYBSCOUPPO-ZRUGTGOESA-N
Formula: C29H46O
SMILES: CC=C(CCC(C)C1CC=C2C3=C(CCC21C)C1(C)CCC(O)CC1CC3)C(C)C
Mol. weight [g/mol]: 410.67

Physical Properties

Property code	Value	Unit	Source
gf	318.11	kJ/mol	Joback Method
hf	-345.56	kJ/mol	Joback Method
hfus	38.59	kJ/mol	Joback Method
hvap	96.56	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.009		Crippen Method
mcvol	369.000	ml/mol	McGowan Method
pc	1035.23	kPa	Joback Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook
tb	1015.64	K	Joback Method
tc	1247.64	K	Joback Method
tf	565.17	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1395.22	J/mol×K	1015.64	Joback Method
cpg	1429.23	J/mol×K	1054.31	Joback Method
cpg	1464.73	J/mol×K	1092.97	Joback Method
cpg	1502.12	J/mol×K	1131.64	Joback Method
cpg	1541.81	J/mol×K	1170.31	Joback Method
cpg	1584.17	J/mol×K	1208.97	Joback Method
cpg	1629.62	J/mol×K	1247.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214725&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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