24-Ethylcholesta-7,22,25-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: IMWBKGMKWXIXEQ-PCWKWJMOSA-N
Formula: C29H46O
SMILES: C=C(C)C(C=CC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C)CC
Mol. weight [g/mol]: 410.67

Physical Properties

Property code	Value	Unit	Source
gf	379.83	kJ/mol	Joback Method
hf	-295.65	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	93.66	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.721		Crippen Method
mcvol	369.000	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	3295.00		NIST Webbook
tb	993.86	K	Joback Method
tc	1223.19	K	Joback Method
tf	529.13	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.74	J/mol×K	993.86	Joback Method
cpg	1431.80	J/mol×K	1032.08	Joback Method
cpg	1465.99	J/mol×K	1070.30	Joback Method
cpg	1501.69	J/mol×K	1108.52	Joback Method
cpg	1539.28	J/mol×K	1146.75	Joback Method
cpg	1579.16	J/mol×K	1184.97	Joback Method
cpg	1621.70	J/mol×K	1223.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214710&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