4-«alpha»-Methyl-24-ethylcholest-8,14-dien-3-«be

Inchi: InChI=1S/C30H50O/c1-8-22(19(2)3)10-9-20(4)24-13-14-26-23-11-12-25-21(5)28(31)16-1
InchiKey: IFKRHDMELMNDNT-GVLRPNHNSA-N
Formula: C30H50O
SMILES: CCC(CCC(C)C1CC=C2C3=C(CCC21C)C1(C)CCC(O)C(C)C1CC3)C(C)C
Mol. weight [g/mol]: 426.72

Physical Properties

Property code	Value	Unit	Source
gf	244.71	kJ/mol	Joback Method
hf	-499.25	kJ/mol	Joback Method
hfus	39.84	kJ/mol	Joback Method
hvap	98.05	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	8.335		Crippen Method
mcvol	387.390	ml/mol	McGowan Method
pc	926.11	kPa	Joback Method
rinpol	3360.00		NIST Webbook
rinpol	3360.00		NIST Webbook
tb	1029.37	K	Joback Method
tc	1261.24	K	Joback Method
tf	576.24	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.41	J/mol×K	1029.37	Joback Method
cpg	1532.37	J/mol×K	1068.02	Joback Method
cpg	1568.59	J/mol×K	1106.66	Joback Method
cpg	1606.43	J/mol×K	1145.31	Joback Method
cpg	1646.27	J/mol×K	1183.95	Joback Method
cpg	1688.49	J/mol×K	1222.60	Joback Method
cpg	1733.44	J/mol×K	1261.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R215000&Units=SI

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