4-«alpha»-Methyl-24-ethylcholest-8-en-3-«beta»-o

Inchi: InChI=1S/C30H52O/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: LXJVEVJHTWVTJO-FRDPUWRRSA-N
Formula: C30H52O
SMILES: CCC(CCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)C(C)C1CC3)C(C)C
Mol. weight [g/mol]: 428.73

Physical Properties

Property code	Value	Unit	Source
gf	216.67	kJ/mol	Joback Method
hf	-565.90	kJ/mol	Joback Method
hfus	40.08	kJ/mol	Joback Method
hvap	96.79	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	8.415		Crippen Method
mcvol	391.690	ml/mol	McGowan Method
pc	896.41	kPa	Joback Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		NIST Webbook
tb	1020.56	K	Joback Method
tc	1250.47	K	Joback Method
tf	558.72	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1530.92	J/mol×K	1020.56	Joback Method
cpg	1565.89	J/mol×K	1058.88	Joback Method
cpg	1601.86	J/mol×K	1097.20	Joback Method
cpg	1639.20	J/mol×K	1135.52	Joback Method
cpg	1678.26	J/mol×K	1173.83	Joback Method
cpg	1719.41	J/mol×K	1212.15	Joback Method
cpg	1763.01	J/mol×K	1250.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R215015&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