24-Ethyl-5-«alpha»-cholest-8,14-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: PHLJEYOBUHONQR-PFGIFUPGSA-N
Formula: C29H48O
SMILES: CCC(CCC(C)C1CC=C2C3=C(CCC21C)C1(C)CCC(O)CC1CC3)C(C)C
Mol. weight [g/mol]: 412.69

Physical Properties

Property code	Value	Unit	Source
gf	244.00	kJ/mol	Joback Method
hf	-458.27	kJ/mol	Joback Method
hfus	36.18	kJ/mol	Joback Method
hvap	96.13	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.089		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	1003.35	kPa	Joback Method
rinpol	3315.00		NIST Webbook
rinpol	3315.00		NIST Webbook
tb	1011.16	K	Joback Method
tc	1240.60	K	Joback Method
tf	569.21	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.77	J/mol×K	1011.16	Joback Method
cpg	1456.19	J/mol×K	1049.40	Joback Method
cpg	1490.81	J/mol×K	1087.64	Joback Method
cpg	1527.00	J/mol×K	1125.88	Joback Method
cpg	1565.12	J/mol×K	1164.12	Joback Method
cpg	1605.53	J/mol×K	1202.36	Joback Method
cpg	1648.61	J/mol×K	1240.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214656&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