Saringosterol

Inchi: InChI=1S/C29H48O2/c1-7-29(31,19(2)3)17-12-20(4)24-10-11-25-23-9-8-21-18-22(30)13-
InchiKey: OPGVEUGCNGNPSX-PQCRNTPGSA-N
Formula: C29H48O2
SMILES: C=CC(O)(CCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 428.69

Physical Properties

Property code	Value	Unit	Source
gf	174.18	kJ/mol	Joback Method
hf	-564.06	kJ/mol	Joback Method
hfus	36.79	kJ/mol	Joback Method
hvap	109.00	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	6.916		Crippen Method
mcvol	379.170	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	3465.00		NIST Webbook
tb	1078.77	K	Joback Method
tc	1320.87	K	Joback Method
tf	611.41	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.05	J/mol×K	1078.77	Joback Method
cpg	1563.30	J/mol×K	1119.12	Joback Method
cpg	1603.77	J/mol×K	1159.47	Joback Method
cpg	1646.90	J/mol×K	1199.82	Joback Method
cpg	1693.18	J/mol×K	1240.17	Joback Method
cpg	1743.06	J/mol×K	1280.52	Joback Method
cpg	1797.01	J/mol×K	1320.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R215560&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