Fucosterol

Other names:	Stigmasta-5,24(28)-dien-3-ol, (3«beta»,24E)- Stigmasta-5,24(28)-dien-3«beta»-ol, (E)- trans-24-Ethylidenecholesterol Fucosterin 28-Isofucosterol 24(E)-Ethylidenecholest-5-en-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:	OSELKOCHBMDKEJ-LBMKRXITSA-N
Formula:	C29H48O
SMILES:	CC=C(CCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	412.69
CAS:	17605-67-3

Physical Properties

Property code	Value	Unit	Source
gf	291.99	kJ/mol	Joback Method
hf	-421.08	kJ/mol	Joback Method
hfus	40.29	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.945		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	3280.00		NIST Webbook
rinpol	3273.74		NIST Webbook
rinpol	3280.00		NIST Webbook
rinpol	3305.00		NIST Webbook
tb	997.18	K	Joback Method
tc	1225.65	K	Joback Method
tf	530.89	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1430.05	J/mol×K	997.18	Joback Method
cpg	1463.55	J/mol×K	1035.26	Joback Method
cpg	1498.11	J/mol×K	1073.34	Joback Method
cpg	1534.10	J/mol×K	1111.42	Joback Method
cpg	1571.91	J/mol×K	1149.49	Joback Method
cpg	1611.89	J/mol×K	1187.57	Joback Method
cpg	1654.44	J/mol×K	1225.65	Joback Method

Sources

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=C17605673&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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