«beta»-Sitosterol

Other names:	(-)-«beta»-Sitosterol
	(24R)-Ethylcholest-5-en-3«beta»-ol
	(24R)-Stigmast-5-en-3«beta»-ol
	.beta.-sitosterol
	22,23-Dihydrostigmasterol
	24«alpha»-Ethylcholesterol
	5-Cholesten-24«beta»-ethyl-3«beta»-ol
	Angelicin
	Angelicin (steroid)
	Azuprostat
	Cinchol
	Cupreol
	Harzol
	NSC 18173
	NSC 8096
	Nimbosterol
	Phytosterol
	Prostasal
	Quebrachol
	Rhamnol
	SKF 14463
	Sito-Lande
	Sitosterol
	Sitosterol (24«beta»-ethylcholest-5-en-3«beta»-ol)
	Sitosterol, «beta»
	Stigmast-5-en-3-ol, (3«beta»)-
	Stigmast-5-en-3«beta»-ol
	Stigmasterol, 22,23-dihydro-
	Triastonal
	stigmast-5-en-3.beta.-ol
	«DELTA»5-Stigmasten-3«beta»-ol
	«alpha»-Dihydrofucosterol
	«alpha»-Phytosterol
	«beta»-Sitosterin
Inchi:	InChI=1S/C29H50O/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:	KZJWDPNRJALLNS-YYRRVRNASA-N
Formula:	C29H50O
SMILES:	CCC(CCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	414.71
CAS:	83-46-5

Physical Properties

Property code	Value	Unit	Source
gf	217.88	kJ/mol	Joback Method
hf	-533.79	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	93.90	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	8.025		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	959.10	kPa	Joback Method
rinpol	3230.00		NIST Webbook
rinpol	3215.00		NIST Webbook
rinpol	3197.00		NIST Webbook
rinpol	3173.00		NIST Webbook
rinpol	3228.00		NIST Webbook
rinpol	3194.00		NIST Webbook
rinpol	3243.00		NIST Webbook
rinpol	3214.00		NIST Webbook
rinpol	3201.00		NIST Webbook
rinpol	3215.00		NIST Webbook
rinpol	3201.00		NIST Webbook
rinpol	3198.00		NIST Webbook
rinpol	3199.00		NIST Webbook
rinpol	3202.00		NIST Webbook
rinpol	3203.00		NIST Webbook
rinpol	3204.00		NIST Webbook
rinpol	3203.00		NIST Webbook
rinpol	3197.00		NIST Webbook
rinpol	3187.00		NIST Webbook
rinpol	3203.00		NIST Webbook
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook
rinpol	3193.00		NIST Webbook
rinpol	3193.00		NIST Webbook
tb	992.70	K	Joback Method
tc	1218.50	K	Joback Method
tf	534.93	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.53	J/mol×K	992.70	Joback Method
cpg	1490.57	J/mol×K	1030.33	Joback Method
cpg	1524.41	J/mol×K	1067.97	Joback Method
cpg	1559.38	J/mol×K	1105.60	Joback Method
cpg	1595.82	J/mol×K	1143.23	Joback Method
cpg	1634.10	J/mol×K	1180.87	Joback Method
cpg	1674.54	J/mol×K	1218.50	Joback Method
hsubt	143.80 ± 0.50	kJ/mol	399.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
ss-Sitosterol Solubility in Selected Organic Solvents:	https://www.doi.org/10.1021/je9009909
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=C83465&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsubt:	Enthalpy of sublimation at a given temperature
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