

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 (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:

5779-62-4

Physical Properties

Property code	Value	Unit	Source
hfus	37.88	kJ/mol	Joback Method
hvap	152.51	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.57		Cheméo Relay (1.0)
logp	8.025		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
tb	698.03	K	Cheméo Relay (1.0)
tf	414.09	K	Cheméo Relay (1.0)

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
ss-Sitosterol Solubility in Selected Organic Solvents:	https://www.doi.org/10.1021/je9009909
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5779624&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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