

Stigmast-7-en-3-ol, (3«beta»,5«alpha»)-

Other names:	24-Ethyl-5«alpha»-cholest-7-en-3«beta»-ol Elasterol, 16,17,25,26-tetrahydro- 5«alpha»-Stigmast-7-en-3«beta»-ol 16,17,25,26-Tetrahydroelasterol 7-Stigmasten-3«beta»-ol Schottenol 24«alpha»-Ethyllathosterol 22,23-Dihydrospinasterol Stigmast-7-en-3«beta»-ol, 5«alpha»- (3«beta»,5«alpha»)-Stigmast-7-en-3-ol 5«alpha»-Stigma-7-en-3«beta»-ol Stigmast-7-en-3-ol
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:	YSKVBPGQYRAUQO-LEJAYFLNSA-N
Formula:	C29H50O
SMILES:	CCC(CCC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]:	414.71
CAS:	521-03-9

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	3382.00		NIST Webbook
rinpol	3345.00		NIST Webbook
rinpol	3382.00		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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C521039&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/29-088-3/Stigmast-7-en-3-ol-3-beta-5-alpha.pdf>

Generated by Cheméo on 2024-04-19 17:36:03.628258214 +0000 UTC m=+15837412.548835529.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.