

Stigmastanol

Other names:	Stigmastan-3-ol, (3«beta»)- Stigmastan-3«beta»-ol 24«alpha»-Ethyl-5«alpha»-cholestan-3«beta»-ol Stigmastanol (24«beta»-ethyl-5«alpha»-cholestan-3«beta»-ol) Stigmastan-3-ol stigmastane-3-«beta»-ol
Inchi:	InChI=1S/C29H52O/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:	LGJMUZUPVCAVPU-VXWLMZFXSA-N
Formula:	C29H52O
SMILES:	CCC(CCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	416.72
CAS:	19466-47-8

Physical Properties

Property code	Value	Unit	Source
gf	189.84	kJ/mol	Joback Method
hf	-600.44	kJ/mol	Joback Method
hfus	38.11	kJ/mol	Joback Method
hvap	92.64	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	8.105		Crippen Method
mcvol	381.900	ml/mol	McGowan Method
pc	927.81	kPa	Joback Method
rinpol	3317.40		NIST Webbook
rinpol	3317.40		NIST Webbook
rinpol	3300.00		NIST Webbook
rinpol	3310.00		NIST Webbook
tb	983.89	K	Joback Method
tc	1207.73	K	Joback Method
tf	517.41	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.57	J/mol×K	983.89	Joback Method
cpg	1523.85	J/mol×K	1021.20	Joback Method
cpg	1557.68	J/mol×K	1058.50	Joback Method
cpg	1592.42	J/mol×K	1095.81	Joback Method
cpg	1628.38	J/mol×K	1133.11	Joback Method
cpg	1665.90	J/mol×K	1170.42	Joback Method
cpg	1705.32	J/mol×K	1207.73	Joback Method

Sources

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=C19466478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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