

Stigmasterol

Other names:	Stigmasta-5,22-dien-3-ol, (3«beta»,22E)- Stigmasta-5,22-dien-3«beta»-ol «beta»-Stigmasterol (24S)-5,22-Stigmastadien-3«beta»-ol Stigmasta-5,22-dien-3-ol, (3«beta»)- Stigmasterin 5,22-Cholestadien-24-ethyl-3«beta»-ol «DELTA»5,22-Stigmastadien-3«beta»-ol Stigmasta-5,22-dien-3-ol NSC 8095 Phytosterol I-Stigmasterol (22E)-Stigmasta-5,22-dien-3-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:	HCXVJBMSMIARIN-BASBAMEESA-N
Formula:	C29H48O
SMILES:	CCC(C=CC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	412.69
CAS:	83-48-7

Physical Properties

Property code	Value	Unit	Source
gf	298.10	kJ/mol	Joback Method
hf	-416.57	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	93.86	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	7.801		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	990.75	kPa	Joback Method
rinpol	3138.00		NIST Webbook
rinpol	3191.00		NIST Webbook
rinpol	3164.00		NIST Webbook
rinpol	3213.00		NIST Webbook
rinpol	3148.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3172.00		NIST Webbook

rinpol	3140.00		NIST Webbook
rinpol	3142.00		NIST Webbook
rinpol	3145.00		NIST Webbook
rinpol	3143.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3142.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3148.00		NIST Webbook
rinpol	3166.00		NIST Webbook
rinpol	3145.00		NIST Webbook
rinpol	3172.00		NIST Webbook
rinpol	3166.00		NIST Webbook
rinpol	3148.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3170.00		NIST Webbook
rinpol	3248.60		NIST Webbook
tb	996.86	K	Joback Method
tc	1225.48	K	Joback Method
tf	529.85	K	Joback Method
vc	1.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1430.59	J/mol×K	996.86	Joback Method
cpg	1463.99	J/mol×K	1034.96	Joback Method
cpg	1498.43	J/mol×K	1073.07	Joback Method
cpg	1534.27	J/mol×K	1111.17	Joback Method
cpg	1571.91	J/mol×K	1149.28	Joback Method
cpg	1611.70	J/mol×K	1187.38	Joback Method
cpg	1654.02	J/mol×K	1225.48	Joback Method
hsubt	168.40 ± 1.40	kJ/mol	403.50	NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C83487&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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

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