

Stigmasta-3,5-diene

Inchi:	InChI=1S/C29H48/c1-7-22(20(2)3)12-11-21(4)25-15-16-26-24-14-13-23-10-8-9-18-28(23)
InchiKey:	ICCTZARHLGPHMT-DIWHCLEHSA-N
Formula:	C29H48
SMILES:	CCC(CCC(C)C1CCC2C3CC=C4C=CCCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	396.69
CAS:	79897-80-6

Physical Properties

Property code	Value	Unit	Source
gf	392.37	kJ/mol	Joback Method
hf	-303.44	kJ/mol	Joback Method
hfus	33.94	kJ/mol	Joback Method
hvap	77.82	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	8.830		Crippen Method
mcvol	367.430	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
rinpol	2718.60		NIST Webbook
tb	904.35	K	Joback Method
tc	1129.09	K	Joback Method
tf	479.11	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.87	J/mol×K	904.35	Joback Method
cpg	1358.21	J/mol×K	941.81	Joback Method
cpg	1389.67	J/mol×K	979.26	Joback Method
cpg	1421.59	J/mol×K	1016.72	Joback Method
cpg	1454.34	J/mol×K	1054.18	Joback Method
cpg	1488.24	J/mol×K	1091.63	Joback Method
cpg	1523.66	J/mol×K	1129.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79897806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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