

Stigmastane

Other names:	5«alpha»-Stigmastane «alpha»-Stigmastane (24R)-5«alpha»-Stigmastane Cholestane, 24-ethyl-, (24R)- Stigmastan 1H-Cyclopenta[a]phenanthrene, 17-(4-ethyl-1,5-dimethylhexyl)hexadecahydro-10,13-dimethyl-, 24-ethyl-5-«alpha»-cholestane [8R-[8«alpha»,9«beta»,10«alpha»,13«alpha»,14«beta»,17«alpha»(1R*,4R*)]]-
Inchi:	InChI=1S/C29H52/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:	GKBHKNPLNHL YHT-MFIPXUIISA-N
Formula:	C29H52
SMILES:	CCC(CCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	400.72
CAS:	601-58-1

Physical Properties

Property code	Value	Unit	Source
gf	334.37	kJ/mol	Joback Method
hf	-427.87	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	9.134		Crippen Method
mcvol	376.030	ml/mol	McGowan Method
pc	895.34	kPa	Joback Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
tb	896.38	K	Joback Method
tc	1117.99	K	Joback Method
tf	460.83	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1388.02	J/mol×K	896.38	Joback Method
cpg	1420.71	J/mol×K	933.32	Joback Method
cpg	1453.24	J/mol×K	970.25	Joback Method
cpg	1485.96	J/mol×K	1007.19	Joback Method
cpg	1519.18	J/mol×K	1044.12	Joback Method
cpg	1553.25	J/mol×K	1081.06	Joback Method
cpg	1588.48	J/mol×K	1117.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C601581&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
mccvol:	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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