

Stigmast-4-en-3-one

Other names:	4-Stigmasten-3-one Sitostenone «DELTA»4-Sitosterol-3-one
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:	RUVUHIUYGJBLGI-INQSPIIZSA-N
Formula:	C29H48O
SMILES:	CCC(CCC(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	412.69
CAS:	1058-61-3

Physical Properties

Property code	Value	Unit	Source
gf	239.82	kJ/mol	Joback Method
hf	-498.92	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	8.233		Crippen Method
mcvol	373.300	ml/mol	McGowan Method
pc	945.00	kPa	Joback Method
rinpol	3458.00		NIST Webbook
rinpol	3435.00		NIST Webbook
tb	973.01	K	Joback Method
tc	1207.19	K	Joback Method
tf	546.57	K	Joback Method
vc	1.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1414.77	J/mol×K	973.01	Joback Method
cpg	1447.96	J/mol×K	1012.04	Joback Method
cpg	1481.61	J/mol×K	1051.07	Joback Method
cpg	1516.07	J/mol×K	1090.10	Joback Method

cpg	1551.70	J/mol×K	1129.13	Joback Method
cpg	1588.83	J/mol×K	1168.16	Joback Method
cpg	1627.84	J/mol×K	1207.19	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=C1058613&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
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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