

4,22-Stigmastadiene-3-one

Other names:	(22E)-Stigmasta-4,22-dien-3-one Stigmasta-4,22-dien-3-one
Inchi:	InChI=1S/C29H46O/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:	MKGZDUKUQPPHFM-OZCVYSMVSA-N
Formula:	C29H46O
SMILES:	CCC(C=CC(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]:	410.67
CAS:	20817-72-5

Physical Properties

Property code	Value	Unit	Source
gf	320.04	kJ/mol	Joback Method
hf	-381.70	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	81.73	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	8.009		Crippen Method
mcvol	369.000	ml/mol	McGowan Method
pc	975.95	kPa	Joback Method
rinpol	3399.00		NIST Webbook
rinpol	3399.00		NIST Webbook
tb	977.17	K	Joback Method
tc	1216.33	K	Joback Method
tf	541.49	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1387.87	J/mol×K	977.17	Joback Method
cpg	1421.58	J/mol×K	1017.03	Joback Method
cpg	1456.00	J/mol×K	1056.89	Joback Method
cpg	1491.54	J/mol×K	1096.75	Joback Method
cpg	1528.58	J/mol×K	1136.61	Joback Method

cpg	1567.52	J/mol×K	1176.47	Joback Method
cpg	1608.74	J/mol×K	1216.33	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=C20817725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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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