

Veratraman-11-one, 17,23-epoxy-3-hydroxy-, (3«beta»,23«beta»)-

Other names:	lervin
	Jervine
	Spiro(9H-benzo(a)fluorene-9,2'(3'H)-furo(3,2-b)-pyridin)-11(1H)-one,2,3,3'a,4,4',5',6,6',6a
	17,23«beta»-Epoxy-3«beta»-hydroxyveratraman-11-one
Inchi:	InChI=1S/C27H39NO3/c1-14-11-21-24(28-13-14)16(3)27(31-21)10-8-19-20-6-5-17-12-18
InchiKey:	CLEXYFLHGFJONT-LTAQWEIUSA-N
Formula:	C27H39NO3
SMILES:	CC1=C2C(=O)C3C(CC=C4CC(O)CCC43C)C2CCC12OC1CC(C)CNC1C2C
Mol. weight [g/mol]:	425.60
CAS:	469-59-0

Physical Properties

Property code	Value	Unit	Source
gf	187.65	kJ/mol	Joback Method
hf	-560.78	kJ/mol	Joback Method
hfus	53.93	kJ/mol	Joback Method
hvap	107.60	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.181		Crippen Method
mcvol	340.820	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	3559.00		NIST Webbook
rinpol	3559.00		NIST Webbook
tb	1118.05	K	Joback Method
tc	1375.64	K	Joback Method
tf	807.61	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1440.28	J/mol×K	1118.05	Joback Method
cpg	1479.09	J/mol×K	1160.98	Joback Method
cpg	1520.12	J/mol×K	1203.91	Joback Method

cpg	1563.84	J/mol×K	1246.85	Joback Method
cpg	1610.71	J/mol×K	1289.78	Joback Method
cpg	1661.18	J/mol×K	1332.71	Joback Method
cpg	1715.71	J/mol×K	1375.64	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=C469590&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
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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