Vitispirane

Other names:	Vitispirane I
	Vitispirane II
	2,10,10-trimethyl-6-methylidene-1-oxaspiro[4.5]dec-7-ene
	2,10,10-trimethyl-6-methylene-1-oxaspiro[4.5]dec-7-ene
Inchi:	InChI=1S/C13H20O/c1-10-6-5-8-12(3,4)13(10)9-7-11(2)14-13/h5-6,11H,1,7-9H2,2-4H3
InchiKey:	DUPDJVDPPBFBPL-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	C=C1C=CCC(C)(C)C12CCC(C)O2
Mol. weight [g/mol]:	192.30
CAS:	65416-59-3

Physical Properties

Property code	Value	Unit	Source
gf	109.91	kJ/mol	Joback Method
hf	-170.53	kJ/mol	Joback Method
hfus	13.81	kJ/mol	Joback Method
hvap	47.40	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.466		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1271.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1260.00		NIST Webbook

rinpol	1260.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1281.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1524.00		NIST Webbook
tb	548.48	K	Joback Method
tc	780.54	K	Joback Method
tf	342.64	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.91	J/mol×K	548.48	Joback Method
cpg	451.73	J/mol×K	587.16	Joback Method
cpg	471.06	J/mol×K	625.83	Joback Method
cpg	489.17	J/mol×K	664.51	Joback Method
cpg	506.32	J/mol×K	703.18	Joback Method
cpg	522.78	J/mol×K	741.86	Joback Method
cpg	538.80	J/mol×K	780.54	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=C65416593&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume