

Vitispirane B

Other names:	Vitispirane 2
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/t
InchiKey:	DUPDJVDPPBFBPL-YUZLPWPTSA-N
Formula:	C13H20O
SMILES:	<chem>C=C1C=CCC(C)(C)C12CCC(C)O2</chem>
Mol. weight [g/mol]:	192.30

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	1252.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1511.00		NIST Webbook
ripol	1529.00		NIST Webbook
tb	548.48	K	Joback Method
tc	780.54	K	Joback Method
tf	342.64	K	Joback Method
vc	0.631	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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