trans-Vitispirane

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-WCQYABFASA-N
Formula: C13H20O
SMILES: C=C1C=CCC(C)(C)C12CCC(C)O2
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
ripol	1553.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R302753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume