D-Verbenone

Other names:	(+)-Verbenone (-)-verbenone (1R)-4,6,6-trimethylbicyclo[3.1.1]hept-3-en-2-one (1R-cis)-4,6,6-Trimethylbicyclo(3.1.1)hept-3-en-2-one (1R-cis)-4,6,6-Trimethylbicyclo(3.1.1)hept-3-ene-2-one (1S)-(-)-verbenone (1S,5S)-4,6,6-trimethyl-bicyclo[3.1.1]hept-3-en-2-one (R)-(+)-Verbenone 2-Pinen-4-one, (1R,5R)-(+)- 4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one, (1R,5R)- 4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one, (1R-cis)- Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1R)- Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1R-cis)- NSC 36846 Verbenone Verbenone, (+)- Verbenone, (d)- Verbinone
Inchi:	InChI=1S/C10H14O/c1-6-4-9(11)8-5-7(6)10(8,2)3/h4,7-8H,5H2,1-3H3/t7-,8+/m0/s1
InchiKey:	DCSCXTJOXBUFGB-JGVFFNPUSA-N
Formula:	C10H14O
SMILES:	CC1=CC(=O)C2CC1C2(C)C
Mol. weight [g/mol]:	150.22
CAS:	18309-32-5

Physical Properties

Property code	Value	Unit	Source
gf	27.26	kJ/mol	Joback Method
hf	-206.78	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	41.59	kJ/mol	Joback Method
ie	9.83	eV	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1170.00		NIST Webbook

rinpol	1228.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1170.00		NIST Webbook
tb	500.70	K	NIST Webbook
tc	740.08	K	Joback Method
tf	335.98	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.39	J/mol×K	513.48	Joback Method
cpg	324.08	J/mol×K	551.25	Joback Method
cpg	339.67	J/mol×K	589.01	Joback Method
cpg	354.29	J/mol×K	626.78	Joback Method
cpg	368.08	J/mol×K	664.55	Joback Method
cpg	381.17	J/mol×K	702.31	Joback Method
cpg	393.70	J/mol×K	740.08	Joback Method
hvapt	58.90	kJ/mol	298.15	Thermodynamic study of selected monoterpenes

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18309325&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamic study of selected monoterpenes: https://www.doi.org/10.1016/j.jct.2013.01.009

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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