Fenchone

Other names:	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-
	2-Norbornanone, 1,3,3-trimethyl-
	1,3,3-Trimethyl-2-norbornanone
	1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one
	1,3,3-Trimethylnorcamphor
	Bicyclo[2.2.1]heptane-2-one,1,3,3-trimethyl
	Fenchon
	1,3,3-Trimethyl-2-norcamphanone
	dl-Fenchone
	NSC 122687
	(.+/-.)-Fenchone
	NSC 8896
	3,3-dimethyl-8,9-dinorbornan-2-one
Inchi:	InChI=1S/C10H16O/c1-9(2)7-4-5-10(3,6-7)8(9)11/h7H,4-6H2,1-3H3
InchiKey:	LHXDLQBQYFFVNW-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC12CCC(C1)C(C)(C)C2=O
Mol. weight [g/mol]:	152.23
CAS:	1195-79-5

Physical Properties

Property code	Value	Unit	Source
gf	1.44	kJ/mol	Joback Method
hf	-237.85	kJ/mol	Joback Method
hfus	3.81	kJ/mol	Joback Method
hvap	39.49	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1096.40		NIST Webbook
rinpol	1096.40		NIST Webbook
tb	509.58	K	Joback Method
tc	742.46	K	Joback Method
tf	346.60	K	Joback Method

vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.29	J/mol×K	509.58	Joback Method
cpg	342.61	J/mol×K	548.39	Joback Method
cpg	359.48	J/mol×K	587.21	Joback Method
cpg	375.18	J/mol×K	626.02	Joback Method
cpg	389.96	J/mol×K	664.83	Joback Method
cpg	404.06	J/mol×K	703.65	Joback Method
cpg	417.76	J/mol×K	742.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1195795&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

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
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