D-Fenchone

Other names:	(+)-Fenchone
	(1S)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one
	(S)-Fenchone
	1,3,3-Trimethylbicyclo(2.2.1)heptan-2-one, (1S)-
	2-Norbornanone, 1,3,3-trimethyl-, (+)-
	2-Norbornanone, 1,3,3-trimethyl-, (1S,4R)-(+)-
	2-heptanone, 1,3,3-trimethylbicyclo[2.2.1]-
	2-norbornanone, 1,3,3-trimethyl0, (1S,4R)-(+)-
	Bicyclo(2.2.1)heptan-2-one, 1,3,3-trimethyl-, (1S)-
	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-
	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-, (1S,4R)-
	D(+)-fenchone
	D-(+)-Fenchone
	bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-, (1S)
	d-1,3,3-Trimethyl-2-norbornanone
	d-1,3,3-Trimethyl-2-norcamphanone
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:	4695-62-9

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	51.40 ± 0.10	kJ/mol	NIST Webbook
hvap	51.70 ± 0.10	kJ/mol	NIST Webbook
hvap	51.10 ± 0.10	kJ/mol	NIST Webbook
log10ws	-1.85		Aqueous Solubility Prediction Method
log10ws	-1.85		Estimated Solubility Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method

pc	3082.99	kPa	Joback Method
tb	466.70	K	NIST Webbook
tb	466.35 ± 0.30	K	NIST Webbook
tc	742.46	K	Joback Method
tf	278.52	K	Aqueous Solubility Prediction Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.96	J/mol×K	664.83	Joback Method
cpg	404.06	J/mol×K	703.65	Joback Method
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	417.76	J/mol×K	742.46	Joback Method
hvapt	47.00	kJ/mol	374.50	NIST Webbook
hvapt	48.90	kJ/mol	382.50	NIST Webbook

Sources

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

Thermodynamic properties of chiral fenchones in some solutions at T = 298.15 K: https://www.doi.org/10.1016/j.jct.2010.12.004

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4695629&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume