L-Fenchone

Other names:	(-)-Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-, (1R)-
	(-)-fenchone
	(1R)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-one
	(R)-Fenchone
	1,3,3-Trimethylbicyclo[2.2.1]heptan-2-one-, (1R,4S)-
	1,3,3-trimethylnorbornan-2-one
	2-norbornanone, 1,3,3-trimethyl-, (1R,4S)-(-)-
	L-(-)-Fenchone
	bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-, (1R)
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:	7787-20-4

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
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
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	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	389.96	J/mol×K	664.83	Joback Method
cpg	417.76	J/mol×K	742.46	Joback Method
rhol	940.67	kg/m3	298.15	Excess molar enthalpies of R-fenchone + propan-1-ol or +propan-2-ol. Modeling with COSMO-RS and UNIFAC

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
283.15	101.00	953.27
298.15	101.00	940.67
313.15	101.00	928.04
328.15	101.00	915.39
283.15	20000.00	965.6
283.15	25000.00	968.5
283.15	30000.00	971.3
283.15	35000.00	974.0
283.15	40000.00	976.6
298.15	20000.00	954.0
298.15	25000.00	957.1
298.15	30000.00	960.0
298.15	35000.00	962.9
298.15	40000.00	965.7
313.15	20000.00	942.3
313.15	25000.00	945.6
313.15	30000.00	948.7
313.15	35000.00	951.8
313.15	40000.00	954.7
328.15	20000.00	930.8

328.15	25000.00	934.2
328.15	30000.00	937.6
328.15	35000.00	940.9
328.15	40000.00	944.0

Reference *https://www.doi.org/10.1016/j.jct.2013.09.024*

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7787204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical properties of {R-fenchone + ethanol} at several temperatures and pressures:	https://www.doi.org/10.1016/j.jct.2013.09.024
Excess molar enthalpies of R-fenchone + propan-1-ol or +propan-2-ol. Modeling with COSMO-RS and UNIFAC:	https://www.doi.org/10.1016/j.jct.2015.04.034
Excess molar enthalpies of R-fenchone + butan-1-ol or + pentan-1-ol. Modeling with COSMO-RS and UNIFAC:	https://www.doi.org/10.1016/j.jct.2018.01.005

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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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