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/t7-,10+/m0/s1
InchiKey:	LHXDLQBQYFFVNW-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC12CCC(C1)C(C)(C)C2=O
Mol. weight [g/mol]:	152.24

Physical Properties

Property code	Value	Unit	Source
hf	-213.41	kJ/mol	Cheméo Relay (1.0)
hfus	3.81	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-2.44		Cheméo Relay (1.0)
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
tb	459.80	K	Cheméo Relay (1.0)
tf	358.02	K	Cheméo Relay (1.0)

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
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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126216&Units=SI
Cheméo Relay (1.0):	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermophysical properties of {R-fenchone + ethanol} at several temperatures and pressures:	https://www.doi.org/10.1016/j.jct.2013.09.024
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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