Pentane, 2-methoxy-2,4,4-trimethyl-

Other names:	2-methoxy-2,4,4-trimethylpentane
	methyl 1,1,3,3-tetramethylbutyl ether
Inchi:	InChI=1S/C9H20O/c1-8(2,3)7-9(4,5)10-6/h7H2,1-6H3
InchiKey:	IKZVAPMTXDXWMX-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	COC(C)(C)CC(C)(C)C
Mol. weight [g/mol]:	144.25
CAS:	62108-41-2

Physical Properties

Property code	Value	Unit	Source
gf	-74.42	kJ/mol	Joback Method
hf	-378.81	kJ/mol	Joback Method
hfus	5.43	kJ/mol	Joback Method
hvap	45.30	kJ/mol	NIST Webbook
hvap	45.33	kJ/mol	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.848		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	897.00		NIST Webbook
rinpol	897.00		NIST Webbook
tb	421.28	K	Joback Method
tc	606.03	K	Joback Method
tf	218.26	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.35	J/mol×K	421.28	Joback Method
cpg	319.08	J/mol×K	452.07	Joback Method
cpg	334.95	J/mol×K	482.86	Joback Method
cpg	350.01	J/mol×K	513.66	Joback Method

cpg	364.29	J/mol×K	544.45	Joback Method
cpg	377.82	J/mol×K	575.24	Joback Method
cpg	390.62	J/mol×K	606.03	Joback Method
dvisc	0.0117159	Pa×s	218.26	Joback Method
dvisc	0.0039669	Pa×s	252.10	Joback Method
dvisc	0.0017355	Pa×s	285.93	Joback Method
dvisc	0.0009045	Pa×s	319.77	Joback Method
dvisc	0.0005340	Pa×s	353.61	Joback Method
dvisc	0.0003456	Pa×s	387.44	Joback Method
dvisc	0.0002399	Pa×s	421.28	Joback Method
hvapt	38.50	kJ/mol	399.50	NIST Webbook
pvap	1.34	kPa	308.00	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.19	kPa	277.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.20	kPa	278.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.24	kPa	280.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.28	kPa	283.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.28	kPa	283.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	0.36	kPa	286.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.17	kPa	276.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.41	kPa	289.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.51	kPa	292.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.56	kPa	293.30	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.61	kPa	295.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.75	kPa	298.00	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.74	kPa	298.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.89	kPa	301.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers

pvap	1.02	kPa	303.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	1.07	kPa	304.20	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
pvap	0.39	kPa	288.10	Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers
rhol	792.40	kg/m3	298.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	784.10	kg/m3	308.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)

rhol	776.00	kg/m3	318.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	767.60	kg/m3	328.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	759.20	kg/m3	338.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	750.70	kg/m3	348.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)

rhol	742.10	kg/m3	358.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	733.40	kg/m3	368.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	724.50	kg/m3	378.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	715.50	kg/m3	388.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)

rhol	706.30	kg/m3	398.15	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)
rhol	696.80	kg/m3	408.16	Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4-trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane)

Sources

Determination of Ambient Temperature Vapor Pressures and Vaporization Enthalpies of Branched Ethers:	https://www.doi.org/10.1021/je0255980
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=C62108412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Infinite dilution activity coefficient measurements by inert gas stripping method:	https://www.doi.org/10.1016/j.fluid.2006.02.022
Measurements and modeling for the density of 2-methoxy-2,4,4-trimethylpentane, HE for (methanol + 2-methoxy-2,4,4- trimethylpentane), LLE for (water + 2-methoxy-2,4,4-trimethylpentane) and LLE for (water + methanol + 2-methoxy-2,4,4-trimethylpentane):	https://www.doi.org/10.1016/j.jct.2015.08.011

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume