Methyl propyl ether

Other names:	1-METHOXY-PROPANE
	1-Methoxypropane
	Ether, methyl propyl
	METOPRYL
	Methyl n-propyl ether
	NEOTHYL
	Propane, 1-methoxy-
	Propyl methyl ether
	UN 2612
	n-C3H7OCH3
	«alpha»-Methoxy propane
	Â«alphaÂ»-Methoxy propane
Inchi:	InChI=1S/C4H10O/c1-3-4-5-2/h3-4H2,1-2H3
InchiKey:	VNKYTQGIUYNRMY-UHFFFAOYSA-N
Formula:	C4H10O
SMILES:	CCCOC
Mol. weight [g/mol]:	74.12
CAS:	557-17-5

Physical Properties

Property code	Value	Unit	Source
af	0.2710		KDB
affp	814.90	kJ/mol	NIST Webbook
basg	785.70	kJ/mol	NIST Webbook
chg	-2765.50 ± 1.00	kJ/mol	NIST Webbook
chl	-2737.23	kJ/mol	NIST Webbook
dm	1.20	debye	KDB
gf	-110.00	kJ/mol	KDB
hf	-237.90	kJ/mol	KDB
hf	-238.02 ± 0.85	kJ/mol	NIST Webbook
hf	-237.70 ± 1.10	kJ/mol	NIST Webbook
hfl	-265.96 ± 0.84	kJ/mol	NIST Webbook
hfus	7.30	kJ/mol	Joback Method
hvap	26.91	kJ/mol	Joback Method
ie	9.41 ± 0.07	eV	NIST Webbook
ie	9.73	eV	NIST Webbook

log10ws	-0.39		Estimated Solubility Method
log10ws	-0.51		Aqueous Solubility Prediction Method
logp	1.043		Crippen Method
mcvol	73.090	ml/mol	McGowan Method
pc	3801.00	kPa	KDB
pc	3801.00 ± 4.00	kPa	NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	499.00		NIST Webbook
rinpol	497.00		NIST Webbook
ripol	644.00		NIST Webbook
sg	352.00	J/mol×K	NIST Webbook
sl	262.90	J/mol×K	NIST Webbook
tb	312.20	K	KDB
tb	311.80 ± 1.00	K	NIST Webbook
tb	311.70	K	NIST Webbook
tb	312.20	K	NIST Webbook
tc	476.25 ± 0.20	K	NIST Webbook
tc	476.25	K	KDB
tc	476.30	K	NIST Webbook
tf	157.00	K	KDB
tt	133.97 ± 0.05	K	NIST Webbook
tt	133.97 ± 0.05	K	NIST Webbook
vc	0.274	m3/kmol	KDB
zc	0.2630130		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.51	J/mol×K	449.63	Joback Method
cpg	116.53	J/mol×K	313.34	Joback Method
cpg	123.63	J/mol×K	340.60	Joback Method
cpg	130.58	J/mol×K	367.86	Joback Method
cpg	137.38	J/mol×K	395.12	Joback Method
cpg	144.02	J/mol×K	422.37	Joback Method
cpg	156.84	J/mol×K	476.89	Joback Method
cpl	165.30	J/mol×K	298.15	NIST Webbook
cpl	165.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0001963	Pa×s	313.34	Joback Method
dvisc	0.0025629	Pa×s	157.07	Joback Method

dvisc	0.0012317	Pa×s	183.12	Joback Method
dvisc	0.0007105	Pa×s	209.16	Joback Method
dvisc	0.0004629	Pa×s	235.21	Joback Method
dvisc	0.0003285	Pa×s	261.25	Joback Method
dvisc	0.0002481	Pa×s	287.30	Joback Method
hfust	7.67	kJ/mol	134.00	NIST Webbook
hfust	7.67	kJ/mol	133.97	NIST Webbook
hfust	7.67	kJ/mol	134.00	NIST Webbook
hvapt	29.70	kJ/mol	292.50	NIST Webbook
hvapt	31.00	kJ/mol	311.70	KDB
hvapt	26.75	kJ/mol	312.20	NIST Webbook
hvapt	27.20	kJ/mol	366.00	NIST Webbook
hvapt	26.70	kJ/mol	438.50	NIST Webbook
hvapt	30.70	kJ/mol	297.00	NIST Webbook
hvapt	29.70	kJ/mol	290.50	NIST Webbook
rhol	738.00	kg/m3	293.00	KDB
sfust	57.25	J/mol×K	133.97	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33135e+01
Coeff. B	-1.96855e+03
Coeff. C	-8.53040e+01
Temperature range (K), min.	236.43
Temperature range (K), max.	331.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.97043e+01
Coeff. B	-5.82130e+03
Coeff. C	-1.00118e+01
Coeff. D	1.10139e-05
Temperature range (K), min.	254.15
Temperature range (K), max.	476.20

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1001.mol
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=C557175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1001
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices

sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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