Propane, 2-methoxy-

Other names:	2-METHOXYPROPANE
	Ether, isopropyl methyl
	ISOPROPYL METHYL ETHER
	Isopryl
	Methyl isopropyl ether
	i-C3H7OCH3
Inchi:	InChI=1S/C4H10O/c1-4(2)5-3/h4H,1-3H3
InchiKey:	RMGHERXMTMUMMV-UHFFFAOYSA-N
Formula:	C4H10O
SMILES:	COC(C)C
Mol. weight [g/mol]:	74.12
CAS:	598-53-8

Physical Properties

Property code	Value	Unit	Source
af	0.2660		KDB
affp	826.30	kJ/mol	NIST Webbook
basg	797.10	kJ/mol	NIST Webbook
chg	-2751.10 ± 0.92	kJ/mol	NIST Webbook
gf	-121.00	kJ/mol	KDB
hf	-252.00 ± 0.96	kJ/mol	NIST Webbook
hf	-252.20	kJ/mol	KDB
hfus	3.78	kJ/mol	Joback Method
hvap	26.40 ± 0.10	kJ/mol	NIST Webbook
hvap	26.40	kJ/mol	NIST Webbook
hvap	26.41	kJ/mol	NIST Webbook
hvap	26.78	kJ/mol	NIST Webbook
ie	9.42 ± 0.07	eV	NIST Webbook
ie	9.42	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.45 ± 0.04	eV	NIST Webbook
log10ws	-0.06		Aqueous Solubility Prediction Method
logp	1.041		Crippen Method
mcvol	73.090	ml/mol	McGowan Method
pc	3762.00 ± 4.00	kPa	NIST Webbook
pc	3762.00	kPa	KDB

sg	341.60	J/mol×K	NIST Webbook
sl	253.70	J/mol×K	NIST Webbook
tb	303.92	K	KDB
tb	303.90	K	NIST Webbook
tc	464.48 ± 0.20	K	NIST Webbook
tc	464.48	K	KDB
tc	464.50	K	NIST Webbook
tf	142.07	K	Joback Method
tt	127.93 ± 0.05	K	NIST Webbook
tt	123.06 ± 0.10	K	NIST Webbook
tt	127.93 ± 0.05	K	NIST Webbook
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.25	J/mol×K	312.90	Joback Method
cpg	123.64	J/mol×K	340.84	Joback Method
cpg	130.85	J/mol×K	368.78	Joback Method
cpg	137.91	J/mol×K	396.71	Joback Method
cpg	144.79	J/mol×K	424.65	Joback Method
cpg	151.50	J/mol×K	452.59	Joback Method
cpg	158.04	J/mol×K	480.53	Joback Method
cpl	161.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0001944	Pa×s	312.90	Joback Method
dvisc	0.0018626	Pa×s	170.54	Joback Method
dvisc	0.0050393	Pa×s	142.07	Joback Method
dvisc	0.0005373	Pa×s	227.48	Joback Method
dvisc	0.0003551	Pa×s	255.96	Joback Method
dvisc	0.0002550	Pa×s	284.43	Joback Method
dvisc	0.0009152	Pa×s	199.01	Joback Method
hfust	5.85	kJ/mol	127.30	NIST Webbook
hfust	5.85	kJ/mol	127.30	NIST Webbook
hvapt	26.05	kJ/mol	303.90	NIST Webbook
hvapt	28.80	kJ/mol	287.50	NIST Webbook
hvapt	28.40	kJ/mol	292.50	NIST Webbook
rhol	724.00	kg/m3	288.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45190e+01
Coeff. B	-2.72698e+03
Coeff. C	-2.84640e+01
Temperature range (K), min.	220.08
Temperature range (K), max.	324.64

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.79811e+01
Coeff. B	-5.03717e+03
Coeff. C	-6.52061e+00
Coeff. D	5.22467e-06
Temperature range (K), min.	127.93
Temperature range (K), max.	464.50

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598538&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1002

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

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1002.mol

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

Legend

af: Acentric Factor

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
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