Propane, 1-methoxy-2-methyl-

Other names:	1-METHOXY-2-METHYL PROPANE
	1-Methoxy-2-methyl-propane
	Ether, isobutyl methyl
	ISOBUTYL METHYL ETHER
	METHYL ISOBUTYL OXIDE
	Methyl isobutyl ether
Inchi:	InChI=1S/C5H12O/c1-5(2)4-6-3/h5H,4H2,1-3H3
InchiKey:	ZYVYEJXMYBUCMN-UHFFFAOYSA-N
Formula:	C5H12O
SMILES:	COCC(C)C
Mol. weight [g/mol]:	88.15
CAS:	625-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-116.22	kJ/mol	Joback Method
hf	-284.03	kJ/mol	Joback Method
hfus	6.37	kJ/mol	Joback Method
hvap	30.31	kJ/mol	NIST Webbook
log10ws	-0.76		Crippen Method
logp	1.289		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	556.00		NIST Webbook
rinpol	559.00		NIST Webbook
rinpol	574.00		NIST Webbook
tb	331.70	K	NIST Webbook
tc	504.03	K	Joback Method
tf	153.34	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	198.08	J/mol×K	504.03	Joback Method
cpg	190.26	J/mol×K	475.99	Joback Method
cpg	182.20	J/mol×K	447.95	Joback Method
cpg	173.90	J/mol×K	419.91	Joback Method
cpg	165.37	J/mol×K	391.86	Joback Method
cpg	156.61	J/mol×K	363.82	Joback Method
cpg	147.62	J/mol×K	335.78	Joback Method
dvisc	0.0058560	Pa×s	153.34	Joback Method
dvisc	0.0002086	Pa×s	335.78	Joback Method
dvisc	0.0002758	Pa×s	305.37	Joback Method
dvisc	0.0003877	Pa×s	274.97	Joback Method
dvisc	0.0005934	Pa×s	244.56	Joback Method
dvisc	0.0010248	Pa×s	214.15	Joback Method
dvisc	0.0021208	Pa×s	183.75	Joback Method
hvapt	28.02	kJ/mol	331.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53216e+01
Coeff. B	-3.19318e+03
Coeff. C	-3.33630e+01
Temperature range (K), min.	245.76
Temperature range (K), max.	352.36

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.16689e+01
Coeff. B	-5.63276e+03
Coeff. C	-7.00322e+00
Coeff. D	5.10989e-06
Temperature range (K), min.	160.00
Temperature range (K), max.	497.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1006
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1006.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625445&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume