Propane, 1-ethoxy-

Other names:	1-ETHOXYPROPANE
	Ether, ethyl propyl
	Ethyl n-propyl ether
	Ethyl propyl ether
	PROPYL ETHYL ETHER
	UN 2615
	n-C3H7OC2H5
Inchi:	InChI=1S/C5H12O/c1-3-5-6-4-2/h3-5H2,1-2H3
InchiKey:	NVJUHMXYKCUMQA-UHFFFAOYSA-N
Formula:	C5H12O
SMILES:	CCCOCC
Mol. weight [g/mol]:	88.15
CAS:	628-32-0

Physical Properties

Property code	Value	Unit	Source
af	0.3330		KDB
chl	-3378.97	kJ/mol	NIST Webbook
dm	1.20	debye	KDB
gf	-125.50	kJ/mol	KDB
hf	-272.20 ± 1.20	kJ/mol	NIST Webbook
hfl	-303.60 ± 1.20	kJ/mol	NIST Webbook
hfus	9.89	kJ/mol	Joback Method
hvap	31.39	kJ/mol	NIST Webbook
hvap	31.43 ± 0.11	kJ/mol	NIST Webbook
hvap	31.40	kJ/mol	NIST Webbook
hvap	31.40	kJ/mol	NIST Webbook
hvap	31.40 ± 0.10	kJ/mol	NIST Webbook
hvap	31.57	kJ/mol	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
log10ws	-0.66		Estimated Solubility Method
log10ws	-0.66		Aqueous Solubility Prediction Method
logp	1.433		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3370.00 ± 6.00	kPa	NIST Webbook

pc	3250.00 ± 40.53	kPa	NIST Webbook
pc	3370.00	kPa	KDB
rhoc	260.13 ± 1.76	kg/m3	NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	566.50		NIST Webbook
rinpol	572.10		NIST Webbook
rinpol	590.00		NIST Webbook
sg	388.10	J/mol×K	NIST Webbook
sl	295.00	J/mol×K	NIST Webbook
tb	336.36	K	KDB
tb	336.30	K	NIST Webbook
tb	336.80	K	NIST Webbook
tb	336.40 ± 0.50	K	NIST Webbook
tc	500.20	K	NIST Webbook
tc	500.60 ± 0.50	K	NIST Webbook
tc	500.23 ± 0.20	K	NIST Webbook
tc	500.23	K	KDB
tf	145.60	K	KDB
tf	146.45 ± 0.40	K	NIST Webbook
tf	145.90	K	Aqueous Solubility Prediction Method
tt	145.65 ± 0.05	K	NIST Webbook
vc	0.339	m3/kmol	KDB
zc	0.2746780		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.09	J/mol×K	473.10	Joback Method
cpg	147.83	J/mol×K	336.22	Joback Method
cpg	156.52	J/mol×K	363.60	Joback Method
cpg	164.99	J/mol×K	390.97	Joback Method
cpg	173.24	J/mol×K	418.35	Joback Method
cpg	181.27	J/mol×K	445.73	Joback Method
cpg	196.68	J/mol×K	500.48	Joback Method
cpl	197.50	J/mol×K	298.15	NIST Webbook
cpl	197.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0002124	Pa×s	336.22	Joback Method
dvisc	0.0030953	Pa×s	168.34	Joback Method
dvisc	0.0014407	Pa×s	196.32	Joback Method
dvisc	0.0008115	Pa×s	224.30	Joback Method

dvisc	0.0005192	Pa×s	252.28	Joback Method
dvisc	0.0003631	Pa×s	280.26	Joback Method
dvisc	0.0002710	Pa×s	308.24	Joback Method
hfust	8.39	kJ/mol	145.70	NIST Webbook
hfust	8.39	kJ/mol	145.65	NIST Webbook
hfust	8.39	kJ/mol	145.70	NIST Webbook
hvapt	31.60	kJ/mol	314.00	NIST Webbook
hvapt	28.94	kJ/mol	336.30	NIST Webbook
hvapt	33.00	kJ/mol	311.50	NIST Webbook
hvapt	29.00	kJ/mol	311.50	NIST Webbook
rhol	733.00	kg/m3	293.00	KDB
sfust	57.64	J/mol×K	145.65	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53548e+01
Coeff. B	-3.24200e+03
Coeff. C	-3.48390e+01
Temperature range (K), min.	250.01
Temperature range (K), max.	357.64

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.32471e+02
Coeff. B	-8.24837e+03
Coeff. C	-1.81397e+01
Coeff. D	1.95507e-05
Temperature range (K), min.	145.65
Temperature range (K), max.	500.23

Sources

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628320&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1009.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1009
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
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1009

Legend

af:	Acentric Factor
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
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-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