Propane, 2-ethoxy-

Other names:	(CH3)2CHOC2H5
	2-Ethoxypropane
	Ether, ethyl isopropyl
	Ethyl isopropyl ether
Inchi:	InChI=1S/C5H12O/c1-4-6-5(2)3/h5H,4H2,1-3H3
InchiKey:	XSJVWZAETSBXKU-UHFFFAOYSA-N
Formula:	C5H12O
SMILES:	CCOC(C)C
Mol. weight [g/mol]:	88.15
CAS:	625-54-7

Physical Properties

Property code	Value	Unit	Source
affp	842.70	kJ/mol	NIST Webbook
basg	813.50	kJ/mol	NIST Webbook
gf	-116.22	kJ/mol	Joback Method
hf	-284.03	kJ/mol	Joback Method
hfus	6.37	kJ/mol	Joback Method
hvap	30.04	kJ/mol	NIST Webbook
hvap	30.32	kJ/mol	NIST Webbook
hvap	30.00	kJ/mol	NIST Webbook
ie	9.38 ± 0.07	eV	NIST Webbook
log10ws	-0.55		Aqueous Solubility Prediction Method
logp	1.431		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	555.00		NIST Webbook
rinpol	555.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	550.00		NIST Webbook
tb	326.50 ± 0.50	K	NIST Webbook
tb	327.20	K	NIST Webbook
tb	366.90 ± 2.00	K	NIST Webbook
tc	490.30	K	NIST Webbook
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	28.21	kJ/mol	327.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52698e+01
Coeff. B	-3.13877e+03
Coeff. C	-3.18200e+01
Temperature range (K), min.	241.32
Temperature range (K), max.	347.01

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625547&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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