Propylene oxide

Other names:	(.+/-.)-1,2-Epoxypropane
	(.+/-.)-Methyloxirane
	1,2-Epoxypropane
	1,2-Propylene oxide
	2,3-Epoxypropane
	2-Methyl oxirane
	2-Methyloxiran
	3-Methyl-1,2-epoxypropane
	AD 6
	AD 6 (suspending agent)
	DL-methyloxirane
	Epihydrin
	Epoxypropane
	Ethylene oxide, methyl-
	METHYL OXIRANE
	Methylethylene oxide
	Methyloxacyclopropane
	Methyloxirane
	NCI-C50099
	Oxirane, 2-methyl-
	Oxirane, methyl-
	Oxyde de propylene
	Propane, 1,2-epoxy-
	Propane, epoxy-
	Propene oxide
	Propylene epoxide
	UN 1280
Inchi:	InChI=1S/C3H6O/c1-3-2-4-3/h3H,2H2,1H3
InchiKey:	GOOHAUXETOMSMM-UHFFFAOYSA-N
Formula:	C3H6O
SMILES:	CC1CO1
Mol. weight [g/mol]:	58.08
CAS:	75-56-9

Physical Properties

Property code	Value	Unit	Source

af	0.2690		KDB
affp	803.30	kJ/mol	NIST Webbook
basg	772.70	kJ/mol	NIST Webbook
chl	-1885.00	kJ/mol	NIST Webbook
chl	-1917.40 ± 1.10	kJ/mol	NIST Webbook
chl	-1893.00	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
gf	-25.80	kJ/mol	KDB
hf	-117.10	kJ/mol	NIST Webbook
hf	-94.68 ± 0.63	kJ/mol	NIST Webbook
hf	-92.82	kJ/mol	KDB
hfl	-122.60 ± 0.63	kJ/mol	NIST Webbook
hfl	-145.00	kJ/mol	NIST Webbook
hfus	9.64	kJ/mol	Joback Method
hvap	27.90	kJ/mol	NIST Webbook
hvap	27.90	kJ/mol	NIST Webbook
hvap	28.31	kJ/mol	NIST Webbook
hvap	27.90	kJ/mol	NIST Webbook
ie	10.26	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.22 ± 0.02	eV	NIST Webbook
ie	10.22 ± 0.02	eV	NIST Webbook
ie	10.44	eV	NIST Webbook
log10ws	-0.59		Aqueous Solubility Prediction Method
logp	0.405		Crippen Method
mcvol	48.140	ml/mol	McGowan Method
pc	5440.00 ± 101.32	kPa	NIST Webbook
pc	4922.84 ± 34.47	kPa	NIST Webbook
pc	4920.00	kPa	KDB
rhoc	299.11 ± 5.81	kg/m3	NIST Webbook
rinpol	448.00		NIST Webbook
rinpol	447.00		NIST Webbook
rinpol	447.00		NIST Webbook
rinpol	447.00		NIST Webbook
rinpol	460.00		NIST Webbook
rinpol	477.00		NIST Webbook
sg	287.40 ± 0.84	J/mol×K	NIST Webbook
sl	196.27	J/mol×K	NIST Webbook
sl	194.60	J/mol×K	NIST Webbook
tb	307.70	K	NIST Webbook
tb	307.97 ± 0.40	K	NIST Webbook
tb	308.15 ± 1.50	K	NIST Webbook
tb	308.00 ± 1.00	K	NIST Webbook
tb	307.90 ± 1.00	K	NIST Webbook

tb	307.45	K	NIST Webbook
tb	308.20	K	NIST Webbook
tb	308.00	K	KDB
tc	482.30 ± 1.00	K	NIST Webbook
tc	488.20 ± 5.00	K	NIST Webbook
tc	482.20	K	KDB
tf	161.18	K	Aqueous Solubility Prediction Method
tf	161.02 ± 0.05	K	NIST Webbook
tf	161.22	K	KDB
tf	161.25	K	NIST Webbook
tt	161.22 ± 0.02	K	NIST Webbook
tt	161.25 ± 0.02	K	NIST Webbook
tt	161.22 ± 0.05	K	NIST Webbook
vc	0.186 ± 0.005	m3/kmol	NIST Webbook
vc	0.195 ± 0.002	m3/kmol	NIST Webbook
vc	0.186	m3/kmol	KDB
zc	0.2282520		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	110.26	J/mol×K	481.72	Joback Method
cpg	98.56	J/mol×K	421.72	Joback Method
cpg	104.58	J/mol×K	451.72	Joback Method
cpg	70.70	J/mol×K	301.73	Joback Method
cpg	78.27	J/mol×K	331.73	Joback Method
cpg	85.43	J/mol×K	361.73	Joback Method
cpg	92.19	J/mol×K	391.72	Joback Method
cpl	125.10	J/mol×K	298.15	NIST Webbook
cpl	122.19	J/mol×K	300.00	NIST Webbook
dvisc	0.0002810	Pa×s	257.18	Joback Method
dvisc	0.0002557	Pa×s	279.46	Joback Method
dvisc	0.0002360	Pa×s	301.73	Joback Method
dvisc	0.0005257	Pa×s	168.08	Joback Method
dvisc	0.0004254	Pa×s	190.35	Joback Method
dvisc	0.0003599	Pa×s	212.63	Joback Method
dvisc	0.0003143	Pa×s	234.91	Joback Method
hfust	6.57	kJ/mol	161.25	NIST Webbook
hfust	6.57	kJ/mol	161.30	NIST Webbook
hfust	6.53	kJ/mol	161.20	NIST Webbook

hfust	6.53	kJ/mol	161.22	NIST Webbook
hfust	6.57	kJ/mol	161.30	NIST Webbook
hvapt	30.10	kJ/mol	278.50	NIST Webbook
hvapt	28.20	kJ/mol	303.50	NIST Webbook
hvapt	32.90	kJ/mol	274.50	NIST Webbook
hvapt	26.99	kJ/mol	307.30	KDB
hvapt	27.35	kJ/mol	307.70	NIST Webbook
hvapt	31.60	kJ/mol	266.50	NIST Webbook
hvapt	28.50	kJ/mol	318.50	NIST Webbook
pvap	237.88	kPa	333.15	Isothermal (vapor + liquid) equilibria for the binary mixtures of (propylene oxide + ethanol) and (propylene oxide + 1-propanol) at several temperatures
pvap	86.90	kPa	303.15	Isothermal (vapor + liquid) equilibria for the binary mixtures of (propylene oxide + ethanol) and (propylene oxide + 1-propanol) at several temperatures
pvap	147.85	kPa	318.15	Isothermal (vapor + liquid) equilibria for the binary mixtures of (propylene oxide + ethanol) and (propylene oxide + 1-propanol) at several temperatures
rhol	829.00	kg/m3	293.00	KDB
sfust	40.74	J/mol×K	161.25	NIST Webbook
sfust	40.52	J/mol×K	161.22	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39516e+01
Coeff. B	-2.40980e+03

Coeff. C	-4.89550e+01
Temperature range (K), min.	225.32
Temperature range (K), max.	329.22

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.12879e+01
Coeff. B	-5.89984e+03
Coeff. C	-1.02173e+01
Coeff. D	1.10873e-05
Temperature range (K), min.	161.22
Temperature range (K), max.	482.25

Sources

Effect of anion species on infinite dilution activity coefficients of epoxides in imidazolium-based ionic liquids:	https://www.doi.org/10.1016/j.fluid.2010.01.007
Isothermal (vapor + liquid) equilibria for the binary mixtures of (propylene oxide + ethanol) and (propylene oxide + 1-propanol) at several temperatures:	https://www.doi.org/10.1016/j.jct.2015.02.006
Isothermal Vapor−Liquid Equilibrium and Excess Enthalpy Data for the Binary Systems Propylene Oxide + 2-Methylpentane and Difluoromethane (R32) + Pentafluoroethane (R125):	https://www.doi.org/10.1021/je034253u
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1043
Vapor-liquid equilibria of binary mixtures of propylene oxide witheither ethyl benzene, 2-methylpentane, or 2-methyl-1-pentene:	https://www.doi.org/10.1016/j.fluid.2013.04.008
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1043
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75569&Units=SI

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
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