Trimethylene oxide

Other names:	1,2-epoxypropane
	1,3-EPOXYPROPANE
	1,3-Propylene oxide
	1,3-Trimethylene oxide
	CYCLOOXABUTANE
	NSC 30086
	Oxacyclobutane
	Oxetan
	Oxetane
	Propane, 1,3-epoxy-
	Trimethylenoxid
	«alpha»,«gamma»-Propane oxide
	Â«alphaÂ»,Â«gammaÂ»-Propane oxide
Inchi:	InChI=1S/C3H6O/c1-2-4-3-1/h1-3H2
InchiKey:	AHHWIHXENZJRFG-UHFFFAOYSA-N
Formula:	C3H6O
SMILES:	C1COC1
Mol. weight [g/mol]:	58.08
CAS:	503-30-0

Physical Properties

Property code	Value	Unit	Source
affp	801.30	kJ/mol	NIST Webbook
basg	773.90	kJ/mol	NIST Webbook
chg	-1957.50 ± 0.59	kJ/mol	NIST Webbook
gf	-55.38	kJ/mol	Joback Method
hf	-80.54 ± 0.63	kJ/mol	NIST Webbook
hf	-80.54	kJ/mol	NIST Webbook
hfus	6.47	kJ/mol	Joback Method
hvap	30.21	kJ/mol	NIST Webbook
hvap	29.80	kJ/mol	NIST Webbook
ie	9.65	eV	NIST Webbook
ie	9.68	eV	NIST Webbook
ie	9.67 ± 0.01	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.64 ± 0.05	eV	NIST Webbook

ie	9.65 ± 0.01	eV	NIST Webbook
log10ws	-0.06		Crippen Method
logp	0.407		Crippen Method
mcvol	48.140	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
rinpol	539.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	553.00		NIST Webbook
rinpol	542.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	544.00		NIST Webbook
tb	323.20	K	NIST Webbook
tb	320.70	K	NIST Webbook
tb	320.80	K	NIST Webbook
tb	321.65 ± 0.50	K	NIST Webbook
tb	320.90 ± 1.00	K	NIST Webbook
tc	507.90	K	NIST Webbook
tf	176.15 ± 1.00	K	NIST Webbook
vc	0.174	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	61.20 ± 0.12	J/mol×K	298.15	NIST Webbook
cpg	103.93 ± 0.21	J/mol×K	498.15	NIST Webbook
cpg	99.08 ± 0.20	J/mol×K	473.15	NIST Webbook
cpg	94.05 ± 0.19	J/mol×K	448.15	NIST Webbook
cpg	88.72 ± 0.18	J/mol×K	423.15	NIST Webbook
cpg	83.34 ± 0.17	J/mol×K	398.15	NIST Webbook
cpg	77.84 ± 0.15	J/mol×K	373.15	NIST Webbook
cpg	72.18 ± 0.14	J/mol×K	348.15	NIST Webbook
cpg	66.66 ± 0.13	J/mol×K	323.15	NIST Webbook
cpg	108.65 ± 0.22	J/mol×K	523.15	NIST Webbook
cpl	99.60	J/mol×K	298.00	NIST Webbook
dvisc	0.0009616	Pa×s	216.09	Joback Method
dvisc	0.0014856	Pa×s	192.44	Joback Method
dvisc	0.0003273	Pa×s	310.67	Joback Method
dvisc	0.0005092	Pa×s	263.38	Joback Method
dvisc	0.0006782	Pa×s	239.73	Joback Method
dvisc	0.0025925	Pa×s	168.80	Joback Method
dvisc	0.0004009	Pa×s	287.02	Joback Method

hfust	6.27	kJ/mol	177.50	NIST Webbook
hvapt	28.67	kJ/mol	320.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42723e+01
Coeff. B	-2.80745e+03
Coeff. C	-3.23930e+01
Temperature range (K), min.	233.14
Temperature range (K), max.	345.69

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.48554e+01
Coeff. B	-5.14105e+03
Coeff. C	-6.01475e+00
Coeff. D	4.77029e-06
Temperature range (K), min.	230.00
Temperature range (K), max.	520.00

Sources

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/mol1044.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C503300&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=1044

Legend

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