1,3,5-Trioxane

Other names:	1,3,5-Trioxacyclohexane
	1,3,5-Trioxan
	Aldeform
	Formagene
	Formaldehyde, trimer
	Marvosan
	Metaformaldehyde
	NSC 26347
	Paraformaldehyde
	S-TRIOXANE
	TRIOXYMETHYLENE
	Triformol
	Triossimetilene
	Trioxan
	Trioxane
	Trioxin
	Trioxymethyleen
	Trioxymethylen
	s-Trioxan
	s-Trixane
	sym-Trioxane
Inchi:	InChI=1S/C3H6O3/c1-4-2-6-3-5-1/h1-3H2
InchiKey:	BGJSXRVXTHVRSN-UHFFFAOYSA-N
Formula:	C3H6O3
SMILES:	C1OCOCO1
Mol. weight [g/mol]:	90.08
CAS:	110-88-3

Physical Properties

Property code	Value	Unit	Source
chs	-1515.30	kJ/mol	NIST Webbook
chs	-1515.70 ± 0.30	kJ/mol	NIST Webbook
chs	-1492.00 ± 1.00	kJ/mol	NIST Webbook
chs	-1518.00	kJ/mol	NIST Webbook
gf	-251.82	kJ/mol	Joback Method
hf	-464.00	kJ/mol	NIST Webbook

hf	-465.76 ± 0.50	kJ/mol	NIST Webbook
hf	-489.50	kJ/mol	NIST Webbook
hfs	-546.00 ± 11.00	kJ/mol	NIST Webbook
hfs	-522.30 ± 0.40	kJ/mol	NIST Webbook
hfs	-520.49	kJ/mol	NIST Webbook
hfus	18.23	kJ/mol	Joback Method
hsub	56.60 ± 0.20	kJ/mol	NIST Webbook
hsub	55.60	kJ/mol	NIST Webbook
hsub	56.50	kJ/mol	NIST Webbook
hsub	48.50 ± 2.50	kJ/mol	NIST Webbook
hsub	56.50	kJ/mol	NIST Webbook
hsub	56.20 ± 0.20	kJ/mol	NIST Webbook
hvap	36.54	kJ/mol	Joback Method
ie	10.30	eV	NIST Webbook
ie	10.80	eV	NIST Webbook
ie	10.59 ± 0.05	eV	NIST Webbook
log10ws	0.28		Crippen Method
logp	-0.078		Crippen Method
mcvol	59.880	ml/mol	McGowan Method
pc	5962.94	kPa	Joback Method
rinpol	660.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	658.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1167.00		NIST Webbook
sg	284.90 ± 3.40	J/mol×K	NIST Webbook
ss	133.00	J/mol×K	NIST Webbook
ss	142.89	J/mol×K	NIST Webbook
tb	373.11	K	Joback Method
tc	585.00	K	Joback Method
tf	335.65 ± 1.50	K	NIST Webbook
tt	333.44 ± 0.02	K	NIST Webbook
vc	0.201	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.33	J/mol×K	585.00	Joback Method
cpg	109.71	J/mol×K	373.11	Joback Method
cpg	151.34	J/mol×K	549.69	Joback Method
cpg	143.93	J/mol×K	514.37	Joback Method

cpg	136.06	J/mol×K	479.06	Joback Method
cpg	127.75	J/mol×K	443.74	Joback Method
cpg	118.97	J/mol×K	408.43	Joback Method
cps	111.40	J/mol×K	298.15	NIST Webbook
cps	113.08	J/mol×K	298.15	NIST Webbook
dvisc	0.0010937	Pa×s	320.37	Joback Method
dvisc	0.0030091	Pa×s	267.64	Joback Method
dvisc	0.0005292	Pa×s	373.11	Joback Method
dvisc	0.0017337	Pa×s	294.00	Joback Method
dvisc	0.0136050	Pa×s	214.90	Joback Method
dvisc	0.0058920	Pa×s	241.27	Joback Method
dvisc	0.0007401	Pa×s	346.74	Joback Method
hfust	15.11	kJ/mol	333.44	NIST Webbook
hfust	15.11	kJ/mol	333.40	NIST Webbook
hfust	15.10	kJ/mol	333.40	NIST Webbook
hfust	15.10	kJ/mol	333.40	NIST Webbook
hsubt	57.90	kJ/mol	221.50	NIST Webbook
hvapt	40.00	kJ/mol	357.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47991e+01
Coeff. B	-3.39060e+03
Coeff. C	-5.51110e+01
Temperature range (K), min.	288.76
Temperature range (K), max.	412.48

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.45411e+01
Coeff. B	-7.85949e+03
Coeff. C	-1.01570e+01
Coeff. D	5.95284e-06
Temperature range (K), min.	329.00
Temperature range (K), max.	604.40

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1045
Solubility of Formaldehyde and Trioxane in Aqueous Solutions:	https://www.doi.org/10.1021/je030243h
Solubility of 1,3,5-Trioxane in Methanol, Ethanol, and 2-Propanol:	https://www.doi.org/10.1021/je049978s
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Partial molar volumes of organic solutes in water. XXII. Cyclic ethers at temperatures (298 to 573) K and pressures up to 30 MPa:	https://www.doi.org/10.1016/j.jct.2009.11.005
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1045.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
New Experimental Results for the Vapor-Liquid Equilibrium of the Binary System (Trioxane + Water) and the Ternary System (Formaldehyde + Trioxane + Water):	https://www.doi.org/10.1021/je050015i
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110883&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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

ripol:	Polar retention indices
sg:	Molar entropy at standard conditions
ss:	Solid 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