Paraldehyde

Other names:	1,3,5-Trimethyl-2,4,6-trioxane
	1,3,5-Trioxane, 2,4,6-trimethyl-
	2,4,6-Trimethyl-1,3,5-trioxaan
	2,4,6-Trimethyl-1,3,5-trioxacyclohexane
	2,4,6-Trimethyl-1,3,5-trioxan
	2,4,6-Trimethyl-1,3,5-trioxane
	2,4,6-Trimethyl-s-trioxane
	2,4,6-Trimetil-1,3,5-triossano
	Acetaldehyde trimer
	Elaldehyde
	NSC 9799
	Paraacetaldehyde
	Paracetaldehyde
	Paral
	Paraldehyd
	Paraldeide
	Pcho
	Rcra waste number U182
	Triacetaldehyde
	Trimethyl trioxane
	UN 1264
	acetaldehyde, trimer
	s-Trimethyltrioxymethylene
	s-Trioxane, 2,4,6-trimethyl-
Inchi:	InChI=1S/C6H12O3/c1-4-7-5(2)9-6(3)8-4/h4-6H,1-3H3
InchiKey:	SQYNKIJPMDEDEG-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	CC1OC(C)OC(C)O1
Mol. weight [g/mol]:	132.16
CAS:	123-63-7

Physical Properties

Property code	Value	Unit	Source
chl	-3394.20 ± 2.60	kJ/mol	NIST Webbook
chl	-3389.00	kJ/mol	NIST Webbook
chl	-3390.00 ± 2.00	kJ/mol	NIST Webbook

gf	-249.69	kJ/mol	Joback Method
hf	-636.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-681.80 ± 2.60	kJ/mol	NIST Webbook
hfus	29.21	kJ/mol	Joback Method
hvap	45.80	kJ/mol	NIST Webbook
hvap	41.00 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.088		Crippen Method
mcvol	102.150	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	786.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	786.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	755.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	734.00		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	767.00		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1070.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1069.00		NIST Webbook
sg	374.40 ± 5.00	J/mol×K	NIST Webbook
sl	289.40	J/mol×K	NIST Webbook
tb	401.15 ± 0.50	K	NIST Webbook
tb	397.20 ± 1.50	K	NIST Webbook
tb	395.00 ± 1.00	K	NIST Webbook
tb	397.15 ± 1.00	K	NIST Webbook
tb	396.50 ± 1.00	K	NIST Webbook
tb	397.15	K	NIST Webbook
tc	563.00 ± 4.00	K	NIST Webbook
tf	285.70 ± 0.10	K	NIST Webbook
tf	285.75	K	NIST Webbook
tf	286.00 ± 0.50	K	NIST Webbook
tf	284.15 ± 1.00	K	NIST Webbook
tf	285.65 ± 0.20	K	NIST Webbook
tt	285.70 ± 0.10	K	NIST Webbook
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.56	J/mol×K	427.74	Joback Method
cpg	289.41	J/mol×K	597.97	Joback Method
cpg	277.41	J/mol×K	563.93	Joback Method
cpg	264.82	J/mol×K	529.88	Joback Method
cpg	251.64	J/mol×K	495.83	Joback Method
cpg	237.89	J/mol×K	461.79	Joback Method
cpg	300.83	J/mol×K	632.02	Joback Method
cpl	254.00	J/mol×K	306.60	NIST Webbook
cpl	250.20	J/mol×K	298.00	NIST Webbook
cpl	257.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0011070	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Paraldehyde + Propylene Carbonate at (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0010010	Pa×s	303.15	Densities and Viscosities of Binary Mixtures of Paraldehyde + Propylene Carbonate at (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0011070	Pa×s	298.15	Molecular interactions in (2,4,6-trimethyl-1,3,5-trioxane + n-alkyl acetates) at T=(298.15, 303.15, and 308.15) K
dvisc	0.0010010	Pa×s	303.15	Molecular interactions in (2,4,6-trimethyl-1,3,5-trioxane + n-alkyl acetates) at T=(298.15, 303.15, and 308.15) K

dvisc	0.0009070	Pa×s	308.15	Molecular interactions in (2,4,6-trimethyl-1,3,5-trioxane + n-alkyl acetates) at T=(298.15, 303.15, and 308.15) K
dvisc	0.0009070	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Paraldehyde + Propylene Carbonate at (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0010010	Pa×s	303.15	Excess Molar Volumes and Viscosity Deviations of Binary Mixtures of 2,4,6-Trimethyl-1,3,5-trioxane + Ethanol, 1-Propanol, and 1-Butanol at (298.15, 303.15, and 308.15) K
dvisc	0.0009070	Pa×s	308.15	Excess Molar Volumes and Viscosity Deviations of Binary Mixtures of 2,4,6-Trimethyl-1,3,5-trioxane + Ethanol, 1-Propanol, and 1-Butanol at (298.15, 303.15, and 308.15) K
dvisc	0.0013740	Pa×s	288.15	Densities and Viscosities of Binary Mixtures of Paraldehyde + Propylene Carbonate at (288.15, 293.15, 298.15, 303.15, and 308.15) K
dvisc	0.0012240	Pa×s	293.15	Densities and Viscosities of Binary Mixtures of Paraldehyde + Propylene Carbonate at (288.15, 293.15, 298.15, 303.15, and 308.15) K

dvisc	0.0011070	Pa×s	298.15	Excess Molar Volumes and Viscosity Deviations of Binary Mixtures of 2,4,6-Trimethyl-1,3,5-trioxane + Ethanol, 1-Propanol, and 1-Butanol at (298.15, 303.15, and 308.15) K
hfust	0.26	kJ/mol	142.70	NIST Webbook
hfust	13.52	kJ/mol	285.70	NIST Webbook
hfust	13.52	kJ/mol	285.70	NIST Webbook
hfust	0.77	kJ/mol	147.50	NIST Webbook
hvapt	41.50	kJ/mol	359.50	NIST Webbook
rfi	1.40290		298.15	Viscosities, Ultrasonic Velocities at (288.15 and 298.15) K, and Refractive Indices at (298.15) K of Binary Mixtures of 2,4,6-Trimethyl-1,3,5-trioxane with Dimethyl Carbonate, Diethyl Carbonate, and Propylene Carbonate
sfust	47.32	J/mol×K	285.70	NIST Webbook
sfust	5.24	J/mol×K	147.50	NIST Webbook
sfust	1.81	J/mol×K	142.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47084e+01
Coeff. B	-3.38746e+03
Coeff. C	-6.14290e+01
Temperature range (K), min.	285.75
Temperature range (K), max.	421.91

Sources

Viscosities, Ultrasonic Velocities at (288.15 and 298.15) K, and Refractive Indices at (298.15) K of Binary Mixtures of 2,4,6-Trimethyl-1,3,5-trioxane with Dimethyl Carbonate, Diethyl Carbonate, and Propylene Carbonate at (288.15, 293.15, 298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je050183a
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Densities and Viscosities of Binary Mixtures of Paraldehyde + Propylene Carbonate at (288.15, 293.15, 298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je0496903
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123637&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Molecular interactions in (2,4,6-trimethyl-1,3,5-trioxane + n-alkyl acetates) at T = (298.15, 308.15, and 308.15) K:	https://www.doi.org/10.1016/j.jct.2006.03.014
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Excess Molar Volumes and Viscosity Deviations of Binary Mixtures of 2,4,6-Trimethyl-1,3,5-trioxane + Ethanol, 1-Propanol, and 1-Butanol at (298.15, 303.15, and 308.15) K:	https://www.doi.org/10.1021/je049556i
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid 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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	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