1,3,5,7-Tetroxane

Other names:	1,3,5,7-Tetraoxoacane
	1,3,5,7-Tetroxocane
Inchi:	InChI=1S/C4H8O4/c1-5-2-7-4-8-3-6-1/h1-4H2
InchiKey:	XGJWQNKXTXSVML-UHFFFAOYSA-N
Formula:	C4H8O4
SMILES:	C1OCOCOCO1
Mol. weight [g/mol]:	120.10
CAS:	293-30-1

Physical Properties

Property code	Value	Unit	Source
chs	-2017.50 ± 0.46	kJ/mol	NIST Webbook
gf	-353.72	kJ/mol	Joback Method
hf	-620.24 ± 0.67	kJ/mol	NIST Webbook
hfs	-699.86 ± 0.50	kJ/mol	NIST Webbook
hfus	24.60	kJ/mol	Joback Method
hsub	79.60 ± 0.20	kJ/mol	NIST Webbook
hsub	79.60 ± 0.20	kJ/mol	NIST Webbook
hsub	79.60	kJ/mol	NIST Webbook
hvap	43.62	kJ/mol	Joback Method
log10ws	0.28		Crippen Method
logp	-0.104		Crippen Method
mcvol	79.840	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
sg	345.60 ± 4.60	J/mol×K	NIST Webbook
ss	167.50	J/mol×K	NIST Webbook
tb	431.48	K	Joback Method
tc	659.60	K	Joback Method
tf	245.70	K	Joback Method
tt	385.00 ± 2.00	K	NIST Webbook
vc	0.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.15	J/mol×K	621.58	Joback Method
cpg	213.27	J/mol×K	583.56	Joback Method
cpg	202.76	J/mol×K	545.54	Joback Method
cpg	191.62	J/mol×K	507.52	Joback Method
cpg	179.88	J/mol×K	469.50	Joback Method
cpg	167.52	J/mol×K	431.48	Joback Method
cpg	232.39	J/mol×K	659.60	Joback Method
cps	142.22	J/mol×K	298.15	NIST Webbook
dvisc	0.0252971	Pa×s	245.70	Joback Method
dvisc	0.0003816	Pa×s	431.48	Joback Method
dvisc	0.0005860	Pa×s	400.52	Joback Method
dvisc	0.0009668	Pa×s	369.55	Joback Method
dvisc	0.0017479	Pa×s	338.59	Joback Method
dvisc	0.0035604	Pa×s	307.63	Joback Method
dvisc	0.0085042	Pa×s	276.66	Joback Method
hfust	22.60	kJ/mol	385.00	NIST Webbook
hfust	22.59	kJ/mol	385.00	NIST Webbook
sfust	58.70	J/mol×K	385.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C293301&Units=SI
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
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

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