1,3,6-Trioxocane

Other names:	Diethylene glycol formal
	Diglycol formal
	1,3,6-Trioxacyclooctane
	1,3,6-Trioxocin, tetrahydro-
	l,3,6-Trioxocane
Inchi:	InChI=1S/C5H10O3/c1-3-7-5-8-4-2-6-1/h1-5H2
InchiKey:	AUAGGMPIKOZAJZ-UHFFFAOYSA-N
Formula:	C5H10O3
SMILES:	C1COCOCCO1
Mol. weight [g/mol]:	118.13
CAS:	1779-19-7

Physical Properties

Property code	Value	Unit	Source
chl	-2880.75 ± 0.99	kJ/mol	NIST Webbook
gf	-259.18	kJ/mol	Joback Method
hf	-467.20 ± 1.20	kJ/mol	NIST Webbook
hfl	-516.00 ± 1.20	kJ/mol	NIST Webbook
hfus	19.21	kJ/mol	Joback Method
hvap	48.77	kJ/mol	NIST Webbook
hvap	48.80 ± 0.20	kJ/mol	NIST Webbook
hvap	48.80	kJ/mol	NIST Webbook
hvap	48.77 ± 0.21	kJ/mol	NIST Webbook
ie	9.23	eV	NIST Webbook
log10ws	0.43		Crippen Method
logp	0.007		Crippen Method
mcvol	88.060	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
tb	427.41	K	Joback Method
tc	653.22	K	Joback Method
tf	230.40	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.95	J/mol×K	427.41	Joback Method
cpg	193.11	J/mol×K	465.04	Joback Method
cpg	206.55	J/mol×K	502.68	Joback Method
cpg	219.29	J/mol×K	540.31	Joback Method
cpg	231.33	J/mol×K	577.95	Joback Method
cpg	242.65	J/mol×K	615.58	Joback Method
cpg	253.27	J/mol×K	653.22	Joback Method
dvisc	0.0311861	Pa×s	230.40	Joback Method
dvisc	0.0091718	Pa×s	263.24	Joback Method
dvisc	0.0035387	Pa×s	296.07	Joback Method
dvisc	0.0016512	Pa×s	328.90	Joback Method
dvisc	0.0008848	Pa×s	361.74	Joback Method
dvisc	0.0005260	Pa×s	394.57	Joback Method
dvisc	0.0003388	Pa×s	427.41	Joback Method

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1779197&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas 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
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume