1,3,6-Dioxathiocane

Other names: Formaldehyde, cyclic thiodiethylene acetal
1,3-Dioxa-6-thiacyclooctane
Inchi: InChI=1S/C5H10O2S/c1-3-8-4-2-7-5-6-1/h1-5H2
InchiKey: QLOPHJMYWXXKTM-UHFFFAOYSA-N
Formula: C5H10O2S
SMILES: C1CSCCOCO1
Mol. weight [g/mol]: 134.20
CAS: 2094-92-0

Physical Properties

Property code	Value	Unit	Source
gf	-133.20	kJ/mol	Joback Method
hf	-302.93	kJ/mol	Joback Method
hfus	14.88	kJ/mol	Joback Method
hvap	42.64	kJ/mol	Joback Method
ie	8.67 ± 0.05	eV	NIST Webbook
log10ws	-0.36		Crippen Method
logp	0.724		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
tb	448.29	K	Joback Method
tc	691.93	K	Joback Method
tf	287.28	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.22	J/mol×K	448.29	Joback Method
cpg	208.98	J/mol×K	488.90	Joback Method
cpg	222.88	J/mol×K	529.50	Joback Method
cpg	235.95	J/mol×K	570.11	Joback Method
cpg	248.19	J/mol×K	610.72	Joback Method
cpg	259.60	J/mol×K	651.32	Joback Method

cpg	270.19	J/mol×K	691.93	Joback Method

Sources

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=C2094920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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