1,3,2-Dioxathiane, 2,2-dioxide

Other names:	1,3-Propanediol, cyclic sulfate
	1,3-Propylene sulfate
	Trimethylene sulfate
	1,3-Propanediol, cyclic sulphate
Inchi:	InChI=1S/C3H6O4S/c4-8(5)6-2-1-3-7-8/h1-3H2
InchiKey:	OQYOVYWFXHQYOP-UHFFFAOYSA-N
Formula:	C3H6O4S
SMILES:	O=S1(=O)OCCCO1
Mol. weight [g/mol]:	138.14
CAS:	1073-05-8

Physical Properties

Property code	Value	Unit	Source
gf	-627.50	kJ/mol	Joback Method
hf	-744.55	kJ/mol	Joback Method
hfus	21.15	kJ/mol	Joback Method
hvap	49.66	kJ/mol	Joback Method
log10ws	0.04		Crippen Method
logp	-0.332		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
pc	7509.11	kPa	Joback Method
tb	372.99	K	Joback Method
tc	569.55	K	Joback Method
tf	334.20 ± 2.00	K	NIST Webbook
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.99	J/mol×K	372.99	Joback Method
cpg	157.00	J/mol×K	405.75	Joback Method
cpg	166.53	J/mol×K	438.51	Joback Method
cpg	175.59	J/mol×K	471.27	Joback Method
cpg	184.20	J/mol×K	504.03	Joback Method

cpg	192.34	J/mol×K	536.79	Joback Method
cpg	200.03	J/mol×K	569.55	Joback Method

Sources

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=C1073058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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