

1,2-Oxathiolane, 2,2-dioxide

Other names:	«gamma»-Propane sultone Propane sultone 1-Propanesulfonic acid, 3-hydroxy-, «gamma»-sultone 1,3-Propane sultone 3-Hydroxy-1-propanesulfonic acid, sultone 3-Hydroxy-1-propanesulfonic acid «gamma»-sultone 3-Hydroxy-1-propanesulphonic acid sultone Rcra waste number U193 NSC 42386
Inchi:	InChI=1S/C3H6O3S/c4-7(5)3-1-2-6-7/h1-3H2
InchiKey:	FSSPGSAQUIYDCN-UHFFFAOYSA-N
Formula:	C3H6O3S
SMILES:	O=S1(=O)CCCO1
Mol. weight [g/mol]:	122.14
CAS:	1120-71-4

Physical Properties

Property code	Value	Unit	Source
gf	-529.28	kJ/mol	Joback Method
hf	-606.39	kJ/mol	Joback Method
hfus	15.27	kJ/mol	Joback Method
hvap	44.98	kJ/mol	Joback Method
log10ws	0.12		Crippen Method
logp	-0.263		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
pc	7305.14	kPa	Joback Method
tb	341.77	K	Joback Method
tc	528.32	K	Joback Method
tf	304.33 ± 0.20	K	NIST Webbook
vc	0.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	123.62	J/mol×K	341.77	Joback Method
cpg	133.07	J/mol×K	372.86	Joback Method
cpg	142.05	J/mol×K	403.95	Joback Method
cpg	150.59	J/mol×K	435.05	Joback Method
cpg	158.68	J/mol×K	466.14	Joback Method
cpg	166.35	J/mol×K	497.23	Joback Method
cpg	173.60	J/mol×K	528.32	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=C1120714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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