3,3'-dimethyl-4-oxo-1,2-dithiolane

Inchi: InChI=1S/C5H8OS2/c1-5(2)4(6)3-7-8-5/h3H2,1-2H3
InchiKey: RGBBJHINMRCYLU-UHFFFAOYSA-N
Formula: C5H8OS2
SMILES: CC1(C)SSCC1=O
Mol. weight [g/mol]: 148.25

Physical Properties

Property code	Value	Unit	Source
gf	-20.59	kJ/mol	Joback Method
hf	-117.99	kJ/mol	Joback Method
hfus	3.17	kJ/mol	Joback Method
hvap	41.70	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.729		Crippen Method
mcvol	104.720	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	492.80	K	Joback Method
tc	757.66	K	Joback Method
tf	416.03	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.30	J/mol×K	492.80	Joback Method
cpg	220.28	J/mol×K	536.94	Joback Method
cpg	231.36	J/mol×K	581.09	Joback Method
cpg	241.68	J/mol×K	625.23	Joback Method
cpg	251.38	J/mol×K	669.37	Joback Method
cpg	260.63	J/mol×K	713.52	Joback Method
cpg	269.56	J/mol×K	757.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R489786&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

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