1,3-Oxathiolane, 2,4-dimethyl-, cis-

Inchi: InChI=1S/C5H10OS/c1-4-3-6-5(2)7-4/h4-5H,3H2,1-2H3/t4-,5+/m1/s1
InchiKey: PINHJTSOQKGKFF-UHNVWZDZSA-N
Formula: C5H10OS
SMILES: CC1COC(C)S1
Mol. weight [g/mol]: 118.20
CAS: 52358-78-8

Physical Properties

Property code	Value	Unit	Source
gf	-26.20	kJ/mol	Joback Method
hf	-193.13	kJ/mol	Joback Method
hfus	15.35	kJ/mol	Joback Method
hvap	36.99	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.484		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	399.19	K	Joback Method
tc	613.97	K	Joback Method
tf	262.79	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.65	J/mol×K	399.19	Joback Method
cpg	185.37	J/mol×K	434.99	Joback Method
cpg	197.47	J/mol×K	470.78	Joback Method
cpg	208.94	J/mol×K	506.58	Joback Method
cpg	219.82	J/mol×K	542.38	Joback Method
cpg	230.11	J/mol×K	578.17	Joback Method
cpg	239.83	J/mol×K	613.97	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=C52358788&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
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