cis-2-Ethyl-2,5-dimethyl-1,3-oxathiolane

Inchi: InChI=1S/C7H14OS/c1-4-7(3)8-6(2)5-9-7/h6H,4-5H2,1-3H3
InchiKey: JMORGBZMPQAHJW-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCC1(C)OC(C)CS1
Mol. weight [g/mol]: 146.25
CAS: 38384-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-14.85	kJ/mol	Joback Method
hf	-219.17	kJ/mol	Joback Method
hfus	14.23	kJ/mol	Joback Method
hvap	40.30	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.264		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	445.19	K	Joback Method
tc	664.50	K	Joback Method
tf	309.23	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.89	J/mol×K	445.19	Joback Method
cpg	268.52	J/mol×K	481.74	Joback Method
cpg	283.04	J/mol×K	518.29	Joback Method
cpg	296.56	J/mol×K	554.84	Joback Method
cpg	309.20	J/mol×K	591.40	Joback Method
cpg	321.06	J/mol×K	627.95	Joback Method
cpg	332.26	J/mol×K	664.50	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=C38384702&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