1,3-Oxathiane, 2,2,4,6-tetramethyl-, cis-

Inchi: InChI=1S/C8H16OS/c1-6-5-7(2)10-8(3,4)9-6/h6-7H,5H2,1-4H3/t6-,7+/m0/s1
InchiKey: LPCWYDWZCPIOJH-NKWVEPMBSA-N
Formula: C8H16OS
SMILES: CC1CC(C)SC(C)(C)O1
Mol. weight [g/mol]: 160.28
CAS: 34560-79-7

Physical Properties

Property code	Value	Unit	Source
gf	-26.24	kJ/mol	Joback Method
hf	-266.31	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	42.38	kJ/mol	Joback Method
ie	8.48 ± 0.02	eV	NIST Webbook
log10ws	-2.87		Crippen Method
logp	2.653		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	467.67	K	Joback Method
tc	692.25	K	Joback Method
tf	312.74	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.75	J/mol×K	467.67	Joback Method
cpg	313.73	J/mol×K	505.10	Joback Method
cpg	330.56	J/mol×K	542.53	Joback Method
cpg	346.34	J/mol×K	579.96	Joback Method
cpg	361.18	J/mol×K	617.39	Joback Method
cpg	375.19	J/mol×K	654.82	Joback Method
cpg	388.47	J/mol×K	692.25	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=C34560797&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
ie:	Ionization energy
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