Thiirane, 2,3-dimethyl-, trans-

Other names:	trans-2-Butene Episulfide
	Butane, 2,3-epithio-, trans-
	trans-2-Butene Sulfide
	trans-2,3-Dimethylthiirane
	(E)-2,3-Dimethylthiirane
	2,3-Dimethyl-thiirane (E)
	trans-Dimethylthiirane
Inchi:	InChI=1S/C4H8S/c1-3-4(2)5-3/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey:	ZMJBHCIEMIVIFZ-IMJSIDKUSA-N
Formula:	C4H8S
SMILES:	CC1SC1C
Mol. weight [g/mol]:	88.17
CAS:	5955-98-6

Physical Properties

Property code	Value	Unit	Source
chl	-3290.00 ± 1.00	kJ/mol	NIST Webbook
gf	75.70	kJ/mol	Joback Method
hf	-28.17	kJ/mol	Joback Method
hfl	-30.00 ± 1.00	kJ/mol	NIST Webbook
hfus	8.98	kJ/mol	Joback Method
hvap	29.91	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.510		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	746.00		NIST Webbook
rinpol	688.00		NIST Webbook
tb	340.82	K	Joback Method
tc	537.89	K	Joback Method
tf	231.99	K	Joback Method
vc	0.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.68	J/mol×K	340.82	Joback Method
cpg	125.45	J/mol×K	373.67	Joback Method
cpg	134.70	J/mol×K	406.51	Joback Method
cpg	143.43	J/mol×K	439.36	Joback Method
cpg	151.68	J/mol×K	472.20	Joback Method
cpg	159.48	J/mol×K	505.05	Joback Method
cpg	166.84	J/mol×K	537.89	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5955986&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume