Thiirane, ethenyl-

Other names:	1-Butene, 3,4-epithio-
	Vinylthiiran
	Vinylthiirane
	3,4-Epithio-1-butene
Inchi:	InChI=1S/C4H6S/c1-2-4-3-5-4/h2,4H,1,3H2
InchiKey:	JNUIIZUUNVYHCS-UHFFFAOYSA-N
Formula:	C4H6S
SMILES:	C=CC1CS1
Mol. weight [g/mol]:	86.16
CAS:	5954-75-6

Physical Properties

Property code	Value	Unit	Source
gf	171.25	kJ/mol	Joback Method
hf	117.60	kJ/mol	Joback Method
hfus	6.63	kJ/mol	Joback Method
hvap	29.55	kJ/mol	Joback Method
ie	8.89	eV	NIST Webbook
log10ws	-1.24		Crippen Method
logp	1.288		Crippen Method
mcvol	68.410	ml/mol	McGowan Method
pc	4849.43	kPa	Joback Method
tb	342.17	K	Joback Method
tc	544.62	K	Joback Method
tf	234.47	K	Joback Method
vc	0.243	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	102.03	J/mol×K	342.17	Joback Method
cpg	110.96	J/mol×K	375.91	Joback Method
cpg	119.26	J/mol×K	409.65	Joback Method
cpg	126.99	J/mol×K	443.39	Joback Method

cpg	134.16	J/mol×K	477.13	Joback Method
cpg	140.83	J/mol×K	510.88	Joback Method
cpg	147.02	J/mol×K	544.62	Joback Method
hvapt	38.70	kJ/mol	304.00	NIST Webbook

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=C5954756&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
hvapt:	Enthalpy of vaporization at a given temperature
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

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