Thietane

Other names:	Propane, 1,3-epithio-
	Thiacyclobutane
	Trimethylene sulfide
	Trimethylenesulfide
Inchi:	InChI=1S/C3H6S/c1-2-4-3-1/h1-3H2
InchiKey:	XSROQCDVUIHRSI-UHFFFAOYSA-N
Formula:	C3H6S
SMILES:	C1CSC1
Mol. weight [g/mol]:	74.14
CAS:	287-27-4

Physical Properties

Property code	Value	Unit	Source
affp	834.80	kJ/mol	NIST Webbook
basg	805.00	kJ/mol	NIST Webbook
chl	-2664.30	kJ/mol	NIST Webbook
chl	-2665.20 ± 0.84	kJ/mol	NIST Webbook
gf	70.60	kJ/mol	Joback Method
hf	59.90	kJ/mol	NIST Webbook
hf	61.10 ± 1.30	kJ/mol	NIST Webbook
hfl	24.00 ± 2.00	kJ/mol	NIST Webbook
hfl	25.20 ± 1.20	kJ/mol	NIST Webbook
hfus	2.15	kJ/mol	Joback Method
hvap	35.90 ± 0.20	kJ/mol	NIST Webbook
hvap	35.90	kJ/mol	NIST Webbook
hvap	36.01	kJ/mol	NIST Webbook
hvap	35.80	kJ/mol	NIST Webbook
ie	8.65 ± 0.01	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	8.61	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.61	eV	NIST Webbook
log10ws	-0.86		Crippen Method
logp	1.123		Crippen Method
mcvol	58.620	ml/mol	McGowan Method
pc	5704.58	kPa	Joback Method
rinpol	743.00		NIST Webbook

rinpol	744.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	744.00		NIST Webbook
sl	184.93	J/mol×K	NIST Webbook
tb	367.00 ± 3.00	K	NIST Webbook
tb	368.10	K	NIST Webbook
tb	367.90	K	NIST Webbook
tc	540.19	K	Joback Method
tf	225.68	K	Joback Method
tt	199.91 ± 0.01	K	NIST Webbook
vc	0.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.70	J/mol×K	505.42	Joback Method
cpg	95.74	J/mol×K	401.10	Joback Method
cpg	103.24	J/mol×K	435.87	Joback Method
cpg	110.22	J/mol×K	470.64	Joback Method
cpg	122.73	J/mol×K	540.19	Joback Method
cpg	79.04	J/mol×K	331.55	Joback Method
cpg	87.68	J/mol×K	366.32	Joback Method
cpl	112.59	J/mol×K	294.37	NIST Webbook
hfust	0.67	kJ/mol	176.70	NIST Webbook
hfust	8.24	kJ/mol	199.90	NIST Webbook
hfust	8.24	kJ/mol	199.90	NIST Webbook
hvapt	34.60	kJ/mol	362.50	NIST Webbook
hvapt	36.50	kJ/mol	334.00	NIST Webbook
hvapt	32.32	kJ/mol	368.10	NIST Webbook
sfust	41.25	J/mol×K	199.90	NIST Webbook
sfust	3.77	J/mol×K	176.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43057e+01

Coeff. B	-3.11206e+03
Coeff. C	-4.66510e+01
Temperature range (K), min.	268.65
Temperature range (K), max.	392.95

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.13704e+01
Coeff. B	-6.54879e+03
Coeff. C	-8.42079e+00
Coeff. D	5.83091e-06
Temperature range (K), min.	268.15
Temperature range (K), max.	603.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C287274&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1862

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1862.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity

basg: Gas basicity

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase 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

hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume