Thiirane, methyl-

Other names:	1,2-Epithiopropane
	2-Methylthiacyclopropane
	2-Methylthiirane
	Methylthiirane
	NSC 36643
	NSC 48100
	Propane, 1,2-epithio-
	Propene sulfide
	Propylene episulfide
	Propylene sulfide
	Propylene sulphide
	Thiirane, 2-methyl-
Inchi:	InChI=1S/C3H6S/c1-3-2-4-3/h3H,2H2,1H3
InchiKey:	MBNVSWHUJDDZRH-UHFFFAOYSA-N
Formula:	C3H6S
SMILES:	CC1CS1
Mol. weight [g/mol]:	74.14
CAS:	1072-43-1

Physical Properties

Property code	Value	Unit	Source
affp	833.30	kJ/mol	NIST Webbook
basg	801.50	kJ/mol	NIST Webbook
chl	-2651.60	kJ/mol	NIST Webbook
gf	74.99	kJ/mol	Joback Method
hf	11.00 ± 1.00	kJ/mol	NIST Webbook
hfus	5.32	kJ/mol	Joback Method
hvap	28.00	kJ/mol	Joback Method
ie	8.60 ± 0.20	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	1.122		Crippen Method
mcvol	58.620	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
rinpol	659.00		NIST Webbook

rinpol	637.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	652.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	659.00		NIST Webbook
ripol	915.00		NIST Webbook
ripol	900.00		NIST Webbook
ripol	924.00		NIST Webbook
ripol	875.00		NIST Webbook
ripol	924.00		NIST Webbook
tb	345.70	K	NIST Webbook
tc	520.84	K	Joback Method
tf	224.96	K	Joback Method
vc	0.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	83.33	J/mol×K	322.61	Joback Method
cpg	91.37	J/mol×K	355.65	Joback Method
cpg	98.89	J/mol×K	388.69	Joback Method
cpg	105.92	J/mol×K	421.72	Joback Method
cpg	112.50	J/mol×K	454.76	Joback Method
cpg	118.64	J/mol×K	487.80	Joback Method
cpg	124.38	J/mol×K	520.84	Joback Method
hvapt	34.60	kJ/mol	347.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42819e+01
Coeff. B	-2.87409e+03

Coeff. C	-4.82860e+01
Temperature range (K), min.	253.66
Temperature range (K), max.	371.18

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=C1072431&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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