2H-Thiopyran, tetrahydro-3-methyl-

Other names:	3-Methyltetrahydro-2H-thiopyrane
	3-Methylthiacyclohexane
	3-Methylthiane
	Thiopyran, tetrahydro-3-methyl-
Inchi:	InChI=1S/C6H12S/c1-6-3-2-4-7-5-6/h6H,2-5H2,1H3
InchiKey:	WTPRCAYZVQKROM-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	CC1CCCSC1
Mol. weight [g/mol]:	116.22
CAS:	5258-50-4

Physical Properties

Property code	Value	Unit	Source
gf	63.95	kJ/mol	Joback Method
hf	-67.59	kJ/mol	Joback Method
hfus	6.79	kJ/mol	Joback Method
hvap	35.19	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.150		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	939.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	922.00		NIST Webbook
tb	404.06	K	Joback Method
tc	626.29	K	Joback Method
tf	248.21	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.17	J/mol×K	404.06	Joback Method
cpg	195.45	J/mol×K	441.10	Joback Method
cpg	209.91	J/mol×K	478.14	Joback Method
cpg	223.57	J/mol×K	515.18	Joback Method
cpg	236.46	J/mol×K	552.22	Joback Method
cpg	248.61	J/mol×K	589.25	Joback Method
cpg	260.03	J/mol×K	626.29	Joback Method
hvapt	42.50	kJ/mol	390.50	NIST Webbook
hvapt	40.70	kJ/mol	398.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33673e+01
Coeff. B	-3.36024e+03
Coeff. C	-5.64170e+01
Temperature range (K), min.	313.32
Temperature range (K), max.	473.53

Sources

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
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=C5258504&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume