2H-Thiopyran, tetrahydro-4-methyl-

Other names:	4-Methyltetrahydro-2H-thiopyrane
	4-Methylthiacyclohexane
	4-Methylthiane
	Thiopyran, tetrahydro-4-methyl-
Inchi:	InChI=1S/C6H12S/c1-6-2-4-7-5-3-6/h6H,2-5H2,1H3
InchiKey:	MCSVISNPQJAWJX-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	CC1CCSCC1
Mol. weight [g/mol]:	116.22
CAS:	5161-17-1

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	925.00		NIST Webbook
rinpol	940.00		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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34049e+01
Coeff. B	-3.37112e+03
Coeff. C	-5.68200e+01
Temperature range (K), min.	313.82
Temperature range (K), max.	473.35

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1888.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5161171&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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