2H-Thiopyran, tetrahydro-2-methyl-

Other names:	Tetrahydro-2-methyl-2H-thiopyran
	2-Methylthiane
	2-methyl-thiacyclohexane
	2-Methyltetrahydro-2H-thiopyrane
Inchi:	InChI=1S/C6H12S/c1-6-4-2-3-5-7-6/h6H,2-5H2,1H3
InchiKey:	VLBGYQISAJHVAD-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	CC1CCCCS1
Mol. weight [g/mol]:	116.22
CAS:	5161-16-0

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	-2.22		Crippen Method
logp	2.292		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	902.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	902.00		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	42.10	kJ/mol	386.00	NIST Webbook
hvapt	40.20	kJ/mol	397.00	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=C5161160&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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