4H-Thiopyran-4-one, tetrahydro-

Other names:	1-Thiacyclohexan-4-one
	2,3,5,6-Tetrahydro-4-thiopyranone
	4-Oxotetrahydrothiopyran
	4-Oxothiane
	4-Thiacyclohexanone
	4-Thianone
	4H-tetrahydrothiopyran-4-one
	NSC 41599
	Penthianone
	Tetrahydro-1,4-thiapyrone
	Tetrahydro-1-thio-4-pyrone
	Tetrahydro-1-thio-«gamma»-pyrone
	Tetrahydro-1-thio-Â«gammaÂ»-pyrone
	Tetrahydro-4-thiopyrone
	Tetrahydro-4H-thiapyran-4-one
	Tetrahydro-4H-thiopyran-4-one
	Tetrahydrothia-4-pyranone
	Tetrahydrothiopyran-4-one
Inchi:	InChI=1S/C5H8OS/c6-5-1-3-7-4-2-5/h1-4H2
InchiKey:	OVRJVKCZJCNSOW-UHFFFAOYSA-N
Formula:	C5H8OS
SMILES:	O=C1CCSCC1
Mol. weight [g/mol]:	116.18
CAS:	1072-72-6

Physical Properties

Property code	Value	Unit	Source
chl	-3485.00 ± 2.10	kJ/mol	NIST Webbook
gf	-59.35	kJ/mol	Joback Method
hf	-155.00 ± 2.70	kJ/mol	NIST Webbook
hfus	2.64	kJ/mol	Joback Method
hsub	72.60 ± 1.70	kJ/mol	NIST Webbook
hvap	72.63	kJ/mol	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	1.083		Crippen Method
mcvol	88.370	ml/mol	McGowan Method

pc	4883.38	kPa	Joback Method
rinpol	1011.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1011.00		NIST Webbook
tb	453.67	K	Joback Method
tc	701.30	K	Joback Method
tf	309.40	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.39	J/mol×K	453.67	Joback Method
cpg	178.19	J/mol×K	494.94	Joback Method
cpg	190.36	J/mol×K	536.21	Joback Method
cpg	201.88	J/mol×K	577.49	Joback Method
cpg	212.76	J/mol×K	618.76	Joback Method
cpg	222.98	J/mol×K	660.03	Joback Method
cpg	232.53	J/mol×K	701.30	Joback Method
hsubt	71.70 ± 1.70	kJ/mol	317.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72313e+01
Coeff. B	-5.80715e+03
Temperature range (K), min.	342.73
Temperature range (K), max.	487.19

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072726&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume