THIANE

Other names:	2H-Thiopyran, tetrahydro-
	Pentamethylene sulfide
	Penthiophane
	Tetrahydro-2H-thiopyran
	Tetrahydrothiapyran
	Tetrahydrothiopyran
	Thiacyclohexane
Inchi:	InChI=1S/C5H10S/c1-2-4-6-5-3-1/h1-5H2
InchiKey:	YPWFISCTZQNZAU-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	C1CCSCC1
Mol. weight [g/mol]:	102.20
CAS:	1613-51-0

Physical Properties

Property code	Value	Unit	Source
af	0.1830		Cheméo Relay (1.0)
affp	855.80	kJ/mol	NIST Webbook
basg	826.00	kJ/mol	NIST Webbook
chl	-3892.50 ± 0.71	kJ/mol	NIST Webbook
chl	-3892.50	kJ/mol	NIST Webbook
hf	-63.30	kJ/mol	NIST Webbook
hf	-63.50 ± 1.00	kJ/mol	NIST Webbook
hfl	-106.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-106.20 ± 0.88	kJ/mol	NIST Webbook
hfus	3.13	kJ/mol	Joback Method
hvap	42.80	kJ/mol	NIST Webbook
hvap	42.70	kJ/mol	NIST Webbook
hvap	42.70	kJ/mol	NIST Webbook
ie	8.36	eV	NIST Webbook
ie	8.39	eV	NIST Webbook
ie	8.45	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
logp	1.904		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rhoc	290.24 ± 39.86	kg/m3	NIST Webbook

rinpol	850.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	880.00		NIST Webbook
sl	218.24	J/mol×K	NIST Webbook
tb	414.90	K	NIST Webbook
tb	415.00 ± 0.40	K	NIST Webbook
tc	684.00 ± 22.00	K	NIST Webbook
tf	291.50 ± 0.10	K	NIST Webbook
tf	292.14 ± 0.05	K	NIST Webbook
tt	292.25 ± 0.07	K	NIST Webbook
tt	292.25 ± 0.07	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.67	J/mol×K	385.85	Joback Method
cpg	211.88	J/mol×K	611.11	Joback Method
cpg	201.97	J/mol×K	573.57	Joback Method
cpg	191.38	J/mol×K	536.02	Joback Method
cpg	180.09	J/mol×K	498.48	Joback Method
cpg	168.06	J/mol×K	460.94	Joback Method
cpg	155.26	J/mol×K	423.39	Joback Method
cpl	163.30	J/mol×K	298.15	NIST Webbook
hfust	2.45	kJ/mol	292.30	NIST Webbook
hfust	1.10	kJ/mol	201.40	NIST Webbook
hfust	7.77	kJ/mol	240.00	NIST Webbook
hfust	2.45	kJ/mol	292.30	NIST Webbook
hvapt	39.70	kJ/mol	351.00	NIST Webbook
hvapt	39.70	kJ/mol	351.00	NIST Webbook
hvapt	42.80 ± 0.20	kJ/mol	350.00	NIST Webbook
hvapt	41.40	kJ/mol	376.50	NIST Webbook
hvapt	42.80 ± 0.20	kJ/mol	350.00	NIST Webbook
hvapt	37.20	kJ/mol	365.50	NIST Webbook
hvapt	39.50	kJ/mol	385.00	NIST Webbook
sfust	8.37	J/mol×K	292.30	NIST Webbook
sfust	32.38	J/mol×K	240.00	NIST Webbook
sfust	5.44	J/mol×K	201.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41416e+01
Coeff. B	-3.43363e+03
Coeff. C	-5.43480e+01
Temperature range (K), min.	292.14
Temperature range (K), max.	443.20

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.31491e+01
Coeff. B	-7.85641e+03
Coeff. C	-1.00487e+01
Coeff. D	5.67464e-06
Temperature range (K), min.	302.15
Temperature range (K), max.	657.12

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1876

KDB: https://www.cheric.org/files/research/kdb/mol/mol1876.mol

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1613510&Units=SI

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

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature