

Thiophene, tetrahydro-

Other names:	NSC 5272
	Pennodorant 1013
	TETRAHYDROTHIOPHENE
	TETRAMETHYLENE SULFIDE
	THIOLANE
	THT
	Tetrahydrothiofen
	Tetrahydrothiophen
	Tetramethylene sulphide
	Thiacyclopentane
	Thilane
	Thiofan
	Thiolan
	Thiophane
	UN 2412
Inchi:	InChI=1S/C4H8S/c1-2-4-5-3-1/h1-4H2
InchiKey:	RAOIDOHSFRTOEL-UHFFFAOYSA-N
Formula:	C4H8S
SMILES:	C1CCSC1
Mol. weight [g/mol]:	88.17
CAS:	110-01-0

Physical Properties

Property code	Value	Unit	Source
affp	849.10	kJ/mol	NIST Webbook
basg	819.30	kJ/mol	NIST Webbook
chl	-3246.20 ± 1.30	kJ/mol	NIST Webbook
chl	-3246.80 ± 1.00	kJ/mol	NIST Webbook
gf	66.92	kJ/mol	Joback Method
hf	-34.50 ± 1.50	kJ/mol	NIST Webbook
hf	-33.60 ± 1.20	kJ/mol	NIST Webbook
hfl	-73.10 ± 1.50	kJ/mol	NIST Webbook
hfl	-72.80 ± 1.20	kJ/mol	NIST Webbook
hfus	2.64	kJ/mol	Joback Method
hvap	38.60	kJ/mol	NIST Webbook
hvap	38.80	kJ/mol	NIST Webbook
hvap	39.20	kJ/mol	NIST Webbook

hvap	38.80	kJ/mol	NIST Webbook
hvap	39.46	kJ/mol	NIST Webbook
hvap	39.20 ± 0.30	kJ/mol	NIST Webbook
ie	8.62	eV	NIST Webbook
ie	8.57 ± 0.15	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.62 ± 0.05	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
log10ws	-1.28		Crippen Method
logp	1.513		Crippen Method
mcvol	72.710	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	801.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	806.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	832.50		NIST Webbook
rinpol	806.30		NIST Webbook
rinpol	812.60		NIST Webbook

rinpol	839.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	778.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1109.00		NIST Webbook
sl	207.82	J/mol×K	NIST Webbook
tb	394.05	K	KDB
tc	632.00	K	NIST Webbook
tc	632.00 ± 1.00	K	NIST Webbook
tf	174.35 ± 1.00	K	NIST Webbook
tt	176.98 ± 0.06	K	NIST Webbook
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.58	J/mol×K	576.06	Joback Method
cpg	157.58	J/mol×K	539.83	Joback Method
cpg	149.03	J/mol×K	503.61	Joback Method
cpg	139.88	J/mol×K	467.38	Joback Method
cpg	130.11	J/mol×K	431.15	Joback Method
cpg	119.69	J/mol×K	394.93	Joback Method
cpg	108.58	J/mol×K	358.70	Joback Method
cpl	140.16	J/mol×K	298.15	NIST Webbook
hfust	7.35	kJ/mol	177.00	NIST Webbook
hfust	7.35	kJ/mol	177.00	NIST Webbook
hfust	7.35	kJ/mol	176.98	NIST Webbook
hvapt	37.70	kJ/mol	366.00	NIST Webbook
hvapt	34.66	kJ/mol	394.30	NIST Webbook
hvapt	37.10	kJ/mol	388.50	NIST Webbook

pvap	91.67	kPa	390.38	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K
pvap	102.02	kPa	394.05	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K
pvap	2.10	kPa	293.97	Infinite dilution activity coefficient and vapour liquid equilibrium measurements for dimethylsulphide and tetrahydrothiophene with hydrocarbons
pvap	5.90	kPa	312.87	Infinite dilution activity coefficient and vapour liquid equilibrium measurements for dimethylsulphide and tetrahydrothiophene with hydrocarbons
pvap	7.30	kPa	318.34	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
pvap	81.18	kPa	386.25	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K

pvap	6.70	kPa	318.35	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
pvap	21.40	kPa	346.14	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
pvap	22.20	kPa	346.97	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
pvap	22.50	kPa	346.97	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
pvap	22.20	kPa	347.07	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
pvap	71.89	kPa	382.18	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K
pvap	63.09	kPa	377.89	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K

pvap	52.61	kPa	372.09	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K
pvap	42.29	kPa	365.30	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K
pvap	20.39	kPa	344.79	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K
pvap	32.09	kPa	357.27	Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + o-xylene at 368.15 K and 383.15 K
pvap	6.90	kPa	318.35	Vapor-Liquid Equilibrium for Tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene
sfust	41.54	J/mol×K	176.98	NIST Webbook
tcondl	0.11	W/m×K	318.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine

tcondl	0.12	W/m×K	303.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.12	W/m×K	288.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.12	W/m×K	273.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine
tcondl	0.11	W/m×K	333.15	Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, Hexamethyleneimine, Tetrahydrothiophene, and Tetramethylethylenediamine

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44868e+01
Coeff. B	-3.46209e+03
Coeff. C	-4.21760e+01
Temperature range (K), min.	286.00
Temperature range (K), max.	419.50

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.59655e+01
Coeff. B	-6.72563e+03
Coeff. C	-7.52404e+00

Coeff. D	4.38631e-06
Temperature range (K), min.	343.15
Temperature range (K), max.	631.95

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110010&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor liquid equilibrium for the binary systems tetrahydrothiophene + toluene and tetrahydrothiophene + n-butane at 353.15 K	https://www.doi.org/10.1016/j.fluid.2009.11.017
Vapor liquid equilibrium for tetrahydrothiophene + n-Butane, + trans-2-Butene, + 2-Methylpropane, and + 2-Methylpropene:	https://www.doi.org/10.1021/je800896m
Vapor liquid equilibrium for binary system of tetrahydrothiophene + 2,2,4-trimethylpentane and 2,2,4-trimethylpentane + n-pentane	http://link.springer.com/article/10.1007/BF02311772
Vapor liquid equilibrium of binary system of tetrahydrothiophene + 2,2,4-trimethylpentane and 2,2,4-trimethylpentane + n-pentane at 353.15 K	https://www.doi.org/10.1016/j.fluid.2010.03.022
Vapor liquid equilibrium of binary system of tetrahydrothiophene + 2,2,4-trimethylpentane and 2,2,4-trimethylpentane + n-pentane at 353.15 K	https://www.doi.org/10.1016/j.fluid.2010.03.027
Vapor liquid equilibrium of binary system of tetrahydrothiophene + 2,2,4-trimethylpentane and 2,2,4-trimethylpentane + n-pentane at 353.15 K	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1869
Vapor liquid equilibrium of binary system of tetrahydrothiophene + 2,2,4-trimethylpentane and 2,2,4-trimethylpentane + n-pentane at 353.15 K	https://en.wikipedia.org/wiki/Joback_method
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
Liquid Thermal Conductivities of Acetonitrile, Diethyl Sulfide, N,N-Dimethylethylamine, Tetrahydrothiophene, and Tetramethylethylenediamine:	https://www.doi.org/10.1021/je0498661
	https://www.cheric.org/files/research/kdb/mol/mol1869.mol

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
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
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
ripol:	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
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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