

Thiophene, tetrahydro-3-methyl-

Other names:	3-METHYLTHIACYCLOPENTANE 3-METHYLTHIOLANE 3-Methyltetrahydrothiophene TETRAHYDRO-3-METHYLTHIOPHENE
Inchi:	InChI=1S/C5H10S/c1-5-2-3-6-4-5/h5H,2-4H2,1H3
InchiKey:	DLABLFPCTXRQMY-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	CC1CCSC1
Mol. weight [g/mol]:	102.20
CAS:	4740-00-5

Physical Properties

Property code	Value	Unit	Source
af	0.2460		KDB
chl	-3896.40 ± 0.59	kJ/mol	NIST Webbook
gf	67.63	kJ/mol	Joback Method
hf	-60.54 ± 0.84	kJ/mol	NIST Webbook
hfl	-102.70 ± 0.79	kJ/mol	NIST Webbook
hfus	6.30	kJ/mol	Joback Method
hvap	42.70	kJ/mol	NIST Webbook
hvap	42.10 ± 0.10	kJ/mol	NIST Webbook
hvap	42.10 ± 0.20	kJ/mol	NIST Webbook
hvap	42.20	kJ/mol	NIST Webbook
log10ws	-1.45		Crippen Method
logp	1.759		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	4375.00	kPa	KDB
rinpol	846.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	847.00		NIST Webbook
sl	241.00	J/mol×K	NIST Webbook
tb	411.50	K	KDB
tc	641.20	K	KDB
tf	192.00	K	KDB
tt	192.00 ± 0.02	K	NIST Webbook
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.47	J/mol×K	591.90	Joback Method
cpg	201.87	J/mol×K	556.07	Joback Method
cpg	191.68	J/mol×K	520.24	Joback Method
cpg	180.86	J/mol×K	484.41	Joback Method
cpg	169.39	J/mol×K	448.57	Joback Method
cpg	157.24	J/mol×K	412.74	Joback Method
cpg	144.38	J/mol×K	376.91	Joback Method
cpl	171.80	J/mol×K	298.15	NIST Webbook
hfust	10.37	kJ/mol	192.00	NIST Webbook
hfust	10.37	kJ/mol	192.00	NIST Webbook
hvapt	39.30	kJ/mol	384.00	NIST Webbook
hvapt	39.60	kJ/mol	396.50	NIST Webbook
hvapt	41.30	kJ/mol	373.00	NIST Webbook
rhoI	1011.72	kg/m3	293.10	KDB
sfust	54.01	J/mol×K	192.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39939e+01
Coeff. B	-3.30168e+03
Coeff. C	-5.93180e+01
Temperature range (K), min.	300.21
Temperature range (K), max.	439.59

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.94861e+01
Coeff. B	-7.62626e+03
Coeff. C	-9.51868e+00

Coeff. D	5.70298e-06
Temperature range (K), min.	340.15
Temperature range (K), max.	453.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4740005&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1879
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1879
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid 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
vc:	Critical Volume

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