

Thiourea

Other names:	(NH2)2CS 2-Thiopseudourea 2-Thiourea Isothiourea NSC 5033 Pseudothiourea Pseudourea, 2-thio- Rcra waste number U219 Sulfourea Sulourea THU Thiocarbamide Thiocarbonic acid diamide Thiomocovina Tsizep 34 UN 2877 USAF EK-497 Urea, 2-thio- Urea, thio- «beta»-Thiopseudourea Â«betaÂ»-Thiopseudourea
Inchi:	InChI=1S/CH4N2S/c2-1(3)4/h(H4,2,3,4)
InchiKey:	UMGDCJDMYOKAJW-UHFFFAOYSA-N
Formula:	CH4N2S
SMILES:	NC(N)=S
Mol. weight [g/mol]:	76.12
CAS:	62-56-6

Physical Properties

Property code	Value	Unit	Source
affp	893.70	kJ/mol	NIST Webbook
basg	863.90	kJ/mol	NIST Webbook
chs	-1474.40 ± 2.10	kJ/mol	NIST Webbook
chs	-1488.00 ± 0.80	kJ/mol	NIST Webbook
chs	-1478.03 ± 0.45	kJ/mol	NIST Webbook
gf	207.50	kJ/mol	Joback Method

hf	22.90 ± 1.60	kJ/mol	NIST Webbook
hfs	-90.00	kJ/mol	NIST Webbook
hfs	-89.10 ± 0.50	kJ/mol	NIST Webbook
hfus	13.34	kJ/mol	Joback Method
hsub	112.00 ± 1.50	kJ/mol	NIST Webbook
hsub	112.00 ± 2.00	kJ/mol	NIST Webbook
hsub	112.00 ± 1.50	kJ/mol	NIST Webbook
hsub	111.00 ± 3.00	kJ/mol	NIST Webbook
hsub	107.60	kJ/mol	NIST Webbook
hvap	45.83	kJ/mol	Joback Method
ie	8.41 ± 0.03	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.50 ± 0.05	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.41	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	0.32		Aqueous Solubility Prediction Method
log10ws	0.32		Estimated Solubility Method
logp	-0.811		Crippen Method
mcvol	56.960	ml/mol	McGowan Method
pc	8145.55	kPa	Joback Method
ss	115.80	J/mol×K	NIST Webbook
tb	437.38	K	Joback Method
tc	674.49	K	Joback Method
tf	450.16	K	Measurement and correlation of solubility of thiourea in two solvent mixtures from T = (283.15 to 313.15) K
tf	448.05 ± 0.20	K	NIST Webbook
tf	453.30 ± 0.10	K	NIST Webbook
tf	451.32	K	Aqueous Solubility Prediction Method
tf	452.20 ± 0.50	K	NIST Webbook
vc	0.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.01	J/mol×K	674.49	Joback Method
cpg	99.61	J/mol×K	437.38	Joback Method

cpg	117.41	J/mol×K	634.97	Joback Method
cpg	114.56	J/mol×K	595.45	Joback Method
cpg	111.40	J/mol×K	555.94	Joback Method
cpg	107.89	J/mol×K	516.42	Joback Method
cpg	103.98	J/mol×K	476.90	Joback Method
cps	96.90	J/mol×K	298.15	NIST Webbook
cps	96.90	J/mol×K	298.15	NIST Webbook
hfust	12.60	kJ/mol	452.20	NIST Webbook
hfust	12.60	kJ/mol	452.20	NIST Webbook
hfust	15.64	kJ/mol	444.70	NIST Webbook
hfust	12.55	kJ/mol	452.20	NIST Webbook
hsubt	103.90 ± 0.30	kJ/mol	387.00	NIST Webbook
hsubt	112.00	kJ/mol	298.15	NIST Webbook
hsubt	109.00 ± 2.00	kJ/mol	408.00	NIST Webbook
hsubt	106.60	kJ/mol	381.50	NIST Webbook
rho1	1405.10	kg/m3	298.15	Measurement and Correlation of Densities and Viscosities of Thiourea in Triglycol + Water at Temperatures from (302.85 to 341.45) K
ssubt	375.60	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54303e+01
Coeff. B	-5.00458e+03
Coeff. C	-7.41600e+01
Temperature range (K), min.	454.15
Temperature range (K), max.	854.00

Sources

Measurement and Correlation of Solubility and Thermodynamic Properties of Pure and Binary Solvents of 2-Ethanol + Water and Thiourea in Water:

<https://www.doi.org/10.1021/acs.jced.8b00663>

<https://www.doi.org/10.1021/je800796h>

Measurement and Correlation for Solubility of Thiourea in Triglycol + Water at Temperatures from (283.15 to 357.75) K: NIST Webbook:

<https://www.doi.org/10.1021/je900040n>

The Yaws Handbook of Vapor Pressure: Crippen Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C62566&Units=SI>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Measurement and correlation of solubility of thiourea in two solvent mixtures from T = (283.15 to 313.15) K: Estimated Solubility Method:

<https://www.doi.org/10.1016/j.jct.2015.11.004>

http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Joback Method:

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

Measurement and Correlation of Densities and Viscosities of Thiourea in Aqueous + Water Vapor at Temperatures from (283.15 to 313.15) K: Estimated Solubility Method:

<https://www.doi.org/10.1021/je9007124>

<https://www.doi.org/10.1021/je301203z>

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rho:	Liquid Density
ss:	Solid phase molar entropy at standard conditions
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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