

Hydrazinecarbothioamide

Other names:	Semicarbazide, thio-
	Isothiosemicarbazide
	N-Aminothiurea
	Thiocarbamoylhydrazine
	Thiosemicarbazide
	TSC
	TSZ
	1-Amino-2-Thiourea
	1-Aminothiurea
	2-Thiosemicarbazide
	Semicarbazide, 3-thio-
	USAF EK-1275
	Rcra waste number P116
	Thiocarbamylhydrazine
	NSC 2213
Inchi:	InChI=1S/CH5N3S/c2-1(5)4-3/h3H2,(H3,2,4,5)
InchiKey:	BRWIZMBXBAOCCF-UHFFFAOYSA-N
Formula:	CH5N3S
SMILES:	NNC(N)=S
Mol. weight [g/mol]:	91.14
CAS:	79-19-6

Physical Properties

Property code	Value	Unit	Source
chs	-1735.10 ± 5.00	kJ/mol	NIST Webbook
chs	-1712.43 ± 0.54	kJ/mol	NIST Webbook
gf	296.89	kJ/mol	Joback Method
hf	128.20 ± 1.60	kJ/mol	NIST Webbook
hfs	2.36 ± 0.59	kJ/mol	NIST Webbook
hfs	-23.85	kJ/mol	NIST Webbook
hfs	24.70 ± 5.00	kJ/mol	NIST Webbook
hfus	18.44	kJ/mol	Joback Method
hsub	125.80 ± 1.50	kJ/mol	NIST Webbook
hsub	125.80 ± 1.50	kJ/mol	NIST Webbook
hvap	52.27	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	-1.307		Crippen Method

mvol	66.940	ml/mol	McGowan Method
pc	8340.11	kPa	Joback Method
ss	128.20	J/mol×K	NIST Webbook
ss	128.20	J/mol×K	NIST Webbook
tb	487.55	K	Joback Method
tc	725.74	K	Joback Method
tf	480.65 ± 2.00	K	NIST Webbook
vc	0.221	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.31	J/mol×K	686.04	Joback Method
cpg	130.68	J/mol×K	487.55	Joback Method
cpg	135.89	J/mol×K	527.25	Joback Method
cpg	140.60	J/mol×K	566.95	Joback Method
cpg	144.87	J/mol×K	606.64	Joback Method
cpg	148.76	J/mol×K	646.34	Joback Method
cpg	155.57	J/mol×K	725.74	Joback Method
cps	114.30	J/mol×K	298.15	NIST Webbook
cps	114.30	J/mol×K	298.15	NIST Webbook
cps	110.90	J/mol×K	298.15	NIST Webbook
hsubt	125.80	kJ/mol	298.15	NIST Webbook
ssubt	421.90	J/mol×K	298.15	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C79196&Units=SI>

Legend

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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
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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