Carbonothioic dihydrazide

Other names:	Carbohydrazide, thio-
	Hydrazinecarbohydrazonothioic acid
	Thiocarbazide
	Thiocarbohydrazide
	Thiocarbonic dihydrazide
	Thiocarbonohydrazide
	TCH
	1,3-Diamino-2-thiourea
	USAF EK-7372
	1,3-Diaminothiourea
	NSC 689
Inchi:	InChI=1S/CH6N4S/c2-4-1(6)5-3/h2-3H2,(H2,4,5,6)
InchiKey:	LJTFFORYSFGNCT-UHFFFAOYSA-N
Formula:	CH6N4S
SMILES:	NNC(=S)NN
Mol. weight [g/mol]:	106.15
CAS:	2231-57-4

Physical Properties

Property code	Value	Unit	Source
chs	-1961.05 ± 0.28	kJ/mol	NIST Webbook
gf	386.28	kJ/mol	Joback Method
hf	260.20 ± 3.00	kJ/mol	NIST Webbook
hfs	108.10 ± 3.50	kJ/mol	NIST Webbook
hfus	23.54	kJ/mol	Joback Method
hsub	152.10 ± 3.00	kJ/mol	NIST Webbook
hsub	152.10 ± 3.00	kJ/mol	NIST Webbook
hvap	58.70	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	-1.802		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	8541.72	kPa	Joback Method
tb	537.72	K	Joback Method
tc	775.49	K	Joback Method
tf	407.14	K	Joback Method
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.00	J/mol×K	696.23	Joback Method
cpg	189.10	J/mol×K	735.86	Joback Method
cpg	164.52	J/mol×K	537.72	Joback Method
cpg	170.36	J/mol×K	577.35	Joback Method
cpg	175.69	J/mol×K	616.98	Joback Method
cpg	180.55	J/mol×K	656.60	Joback Method
cpg	192.90	J/mol×K	775.49	Joback Method
cps	125.30	J/mol×K	298.15	NIST Webbook
hsubt	152.10	kJ/mol	298.15	NIST Webbook
ssubt	510.10	J/mol×K	298.15	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2231574&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
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume