1,3,5-Triazine

Other names:	s-Triazine
	Cyanidine
	Vedita 250
	s-Triazine-(1,3,5)
	sym-Triazine
Inchi:	InChI=1S/C3H3N3/c1-4-2-6-3-5-1/h1-3H
InchiKey:	JIHQDMXYYFUGFV-UHFFFAOYSA-N
Formula:	C3H3N3
SMILES:	c1ncncn1
Mol. weight [g/mol]:	81.08
CAS:	290-87-9

Physical Properties

Property code	Value	Unit	Source
affp	848.80	kJ/mol	NIST Webbook
basg	819.60	kJ/mol	NIST Webbook
chl	-1782.60 ± 0.92	kJ/mol	NIST Webbook
chs	-1780.96 ± 0.67	kJ/mol	NIST Webbook
ea	0.45	eV	NIST Webbook
hf	225.87 ± 0.89	kJ/mol	NIST Webbook
hf	224.70 ± 4.60	kJ/mol	NIST Webbook
hfs	171.69 ± 0.77	kJ/mol	NIST Webbook
hsub	56.50 ± 2.10	kJ/mol	NIST Webbook
hsub	54.20 ± 0.20	kJ/mol	NIST Webbook
hsub	54.20	kJ/mol	NIST Webbook
hsub	54.18 ± 0.19	kJ/mol	NIST Webbook
hvap	38.80 ± 1.90	kJ/mol	NIST Webbook
hvap	55.20 ± 0.10	kJ/mol	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.01 ± 0.01	eV	NIST Webbook
ie	9.98	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	10.51	eV	NIST Webbook
ie	10.07 ± 0.05	eV	NIST Webbook
log10ws	-0.77		Crippen Method
logp	-0.128		Crippen Method
mcvol	59.310	ml/mol	McGowan Method

rinpol	663.00		NIST Webbook
rinpol	663.00		NIST Webbook
ss	125.97	J/mol×K	NIST Webbook
tb	387.20	K	NIST Webbook
tt	353.90 ± 0.20	K	NIST Webbook
tt	353.44 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	95.57	J/mol×K	298.15	NIST Webbook
cps	95.60	J/mol×K	298.15	NIST Webbook
hfust	14.56	kJ/mol	353.40	NIST Webbook
hfust	14.56	kJ/mol	353.40	NIST Webbook
hfust	0.07	kJ/mol	197.70	NIST Webbook
hsubt	58.20	kJ/mol	220.50	NIST Webbook
sfust	0.37	J/mol×K	197.70	NIST Webbook
sfust	41.20	J/mol×K	353.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C290879&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
chs: Standard solid enthalpy of combustion
cps: Solid phase heat capacity
ea: Electron affinity
hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation 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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tt:	Triple Point Temperature