Tetramethylbutanedinitrile

Other names:	Tetramethylsuccinonitrile
	Butanedinitrile, tetramethyl-
	Succinonitrile, tetramethyl-
	Tetramethylsuccinodinitrile
	Tetramethylsuccinotrile
	Tetramethylsuccinic acid dinitrile
	Tetramethylsukcinonitril
	TMSN
	2,3-Dicyano-2,3-dimethylbutane
	2,2,3,3-Tetramethylbutanedinitrile
	NSC 39746
	Butanedinitrile, 2,2,3,3-tetramethyl-
Inchi:	InChI=1S/C8H12N2/c1-7(2,5-9)8(3,4)6-10/h1-4H3
InchiKey:	ZVQXQPNJHRNGID-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CC(C)(C#N)C(C)(C)C#N
Mol. weight [g/mol]:	136.19
CAS:	3333-52-6

Physical Properties

Property code	Value	Unit	Source
chs	-4878.00 ± 1.30	kJ/mol	NIST Webbook
gf	288.52	kJ/mol	Joback Method
hf	100.60	kJ/mol	NIST Webbook
hf	101.00 ± 2.00	kJ/mol	NIST Webbook
hfs	14.90 ± 1.30	kJ/mol	NIST Webbook
hfs	19.90 ± 0.63	kJ/mol	NIST Webbook
hfus	4.66	kJ/mol	Joback Method
hsub	85.69	kJ/mol	NIST Webbook
hsub	81.10	kJ/mol	NIST Webbook
hsub	81.00 ± 2.00	kJ/mol	NIST Webbook
hsub	85.70	kJ/mol	NIST Webbook
hvap	51.77	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.086		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method

tb	580.14	K	Joback Method
tc	807.41	K	Joback Method
tf	442.20 ± 2.00	K	NIST Webbook
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.92	J/mol×K	580.14	Joback Method
cpg	313.77	J/mol×K	618.02	Joback Method
cpg	323.78	J/mol×K	655.90	Joback Method
cpg	333.02	J/mol×K	693.77	Joback Method
cpg	341.55	J/mol×K	731.65	Joback Method
cpg	349.45	J/mol×K	769.53	Joback Method
cpg	356.79	J/mol×K	807.41	Joback Method
hfust	7.15	kJ/mol	442.00	NIST Webbook
hfust	18.10	kJ/mol	345.00	NIST Webbook
hfust	7.15	kJ/mol	442.00	NIST Webbook
sfust	52.48	J/mol×K	345.00	NIST Webbook
sfust	16.17	J/mol×K	442.00	NIST Webbook

Sources

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=C3333526&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume