Hexahydro-1,3,5-trinitroso-1,3,5-triazine

Other names:	1,3,5-Triazine, hexahydro-1,3,5-trinitroso-
	1,3,5-Trinitroso-1,3,5-triazine, hexahydro-
	1,3,5-Trinitrosohexahydro-s-triazine
	1,3,5-trinitroso-1,3,5-triazacyclohexane
	Hexahydro-1,3,5-s-triazine
	Hexahydro-1,3,5-trinitroso-s-triazine
	N,N',N''-Trinitroso-1,3,5-hexahydrotriazine
	TNOHX
	TTT
	Trinitrosotrimethylenetriamine
	Trinitrosotrimethylentriamin
	s-triazine, hexahydro-1,3,5-trinitroso-
Inchi:	InChI=1S/C3H6N6O3/c10-4-7-1-8(5-11)3-9(2-7)6-12/h1-3H2
InchiKey:	HFWOSHMLDRSIDN-UHFFFAOYSA-N
Formula:	C3H6N6O3
SMILES:	O=NN1CN(N=O)CN(N=O)C1
Mol. weight [g/mol]:	174.12
CAS:	13980-04-6

Physical Properties

Property code	Value	Unit	Source
chs	-2316.00	kJ/mol	NIST Webbook
chs	-2313.30 ± 2.10	kJ/mol	NIST Webbook
chs	-2323.90	kJ/mol	NIST Webbook
chs	-2323.90 ± 2.30	kJ/mol	NIST Webbook
hf	395.00	kJ/mol	NIST Webbook
hfs	286.00	kJ/mol	NIST Webbook
hfs	285.90 ± 2.30	kJ/mol	NIST Webbook
hsub	134.30 ± 0.70	kJ/mol	NIST Webbook
hsub	113.00	kJ/mol	NIST Webbook
log10ws	-1.72		Crippen Method
logp	-0.177		Crippen Method
mcvol	106.860	ml/mol	McGowan Method
tf	376.00 ± 1.00	K	NIST Webbook

tt	369.25	K	Thermal behavior of 1,3,5-trinitroso-1,3,5-triazinane and its melt-castable mixtures with cyclic nitramines

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	3.77	kJ/mol	376.00	NIST Webbook
hfust	17.78	kJ/mol	367.00	NIST Webbook
hfust	3.77	kJ/mol	376.00	NIST Webbook
hsubt	112.10	kJ/mol	397.00	NIST Webbook
sfust	48.45	J/mol×K	367.00	NIST Webbook
sfust	10.02	J/mol×K	376.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13980046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal behavior of 1,3,5-trinitroso-1,3,5-triazinane and its melt-castable mixtures with cyclic nitramines:	https://www.doi.org/10.1016/j.tca.2015.07.010
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
tf:	Normal melting (fusion) point

tt: Triple Point Temperature

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