Isothiocyanic acid, hexamethylene ester

Other names:	1,6-Diisothiocyanatohexane
	Hexane, 1,6-diisothiocyanato-
	Isothiocyanic acid, hexamethylene diester
Inchi:	InChI=1S/C8H12N2S2/c11-7-9-5-3-1-2-4-6-10-8-12/h1-6H2
InchiKey:	VZZPYUKWXDLMGI-UHFFFAOYSA-N
Formula:	C8H12N2S2
SMILES:	S=C=NCCCCCCN=C=S
Mol. weight [g/mol]:	200.32
CAS:	5586-70-9

Physical Properties

Property code	Value	Unit	Source
hf	359.69	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.752		Crippen Method
mcvol	159.040	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	674.34	K	Joback Method
tc	919.69	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5586709&Units=SI
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

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature