N-Cyano-S,S'-dimethyldithioimido carbonate

Other names:	Dimethyl cyanodithioiminocarbonate
	Dimethyl N-cyanodithioiminocarbonate
	S,S'-Dimethyl N-cyanodithioiminocarbonate
	Carbonimidodithioic acid, cyano-, dimethyl ester
	(Cyanoimino)bis(methylthio)methane
	Cyanodithioimidocarbonic acid, dimethyl ester
	Dimethyl cyanimidodithiocarbonate
	Dimethyl cyanocarbonimidodithioate
	Dimethyl cyanoiminodithiocarbonate
	Dimethyl N-cyanoimidodithiocarbonate
	Imidocarbonic acid, cyanodithio-, dimethyl ester
	S,S-Dimethyl (N-cyanoimido)dithiocarbonate
	S,S-Dimethyl cyaniminodithiocarbamate
	Carbonimidodithioic acid, N-cyano-, dimethyl ester
	NSC 145987
	S,S-Dimethyl cyanoimidodithiocarbonate
Inchi:	InChI=1S/C4H6N2S2/c1-7-4(8-2)6-3-5/h1-2H3
InchiKey:	IULFXBLVJIPESI-UHFFFAOYSA-N
Formula:	C4H6N2S2
SMILES:	CSC(=NC#N)SC
Mol. weight [g/mol]:	146.23
CAS:	10191-60-3

Physical Properties

Property code	Value	Unit	Source
hf	195.16	kJ/mol	Joback Method
hvap	52.00	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	9.40 ± 0.05	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.549		Crippen Method
mcvol	106.980	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	607.12	K	Joback Method
tc	868.96	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10191603&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature