Methane, isothiocyanato-

Other names:	Isothiocyanic acid, methyl ester
	Isothiocyanatomethane
	Methyl isothiocyanate
	Methyl mustard oil
	Methyl thioisocyanate
	Morton EP-161E
	Trapex
	Trapexide
	Tropex
	WN 12
	CH3NCS
	EP-161E
	Isothiocyanate de methyle
	Isotiocianato di metile
	Methylisothiocyanaat
	Methyl-isothiocyanat
	Methylisothiokyanat
	Methylsenfoel
	MIT
	Mitc
	UN 2477
	Vorlex (Nor-Am)
	Vortex
	Biomet 33
	Degussa methyl isothiocyanate
	MeNCS
	Methane isothiocyanate
	Methyl mustard
Inchi:	InChI=1S/C2H3NS/c1-3-2-4/h1H3
InchiKey:	LGDSHSYDSCRFAB-UHFFFAOYSA-N
Formula:	C2H3NS
SMILES:	CN=C=S
Mol. weight [g/mol]:	73.12
CAS:	556-61-6

Physical Properties

Property code	Value	Unit	Source

affp	799.20	kJ/mol	NIST Webbook
basg	766.70	kJ/mol	NIST Webbook
chs	-1897.40	kJ/mol	NIST Webbook
hf	199.46	kJ/mol	Joback Method
hfs	79.60 ± 1.30	kJ/mol	NIST Webbook
hvap	37.30	kJ/mol	NIST Webbook
ie	9.13 ± 0.15	eV	NIST Webbook
ie	9.37 ± 0.02	eV	NIST Webbook
ie	9.25 ± 0.03	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.719		Crippen Method
mcvol	56.770	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
rinpol	689.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	725.60		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	709.00		NIST Webbook
rinpol	742.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1228.00		NIST Webbook
ripol	1243.00		NIST Webbook
tb	391.11	K	Joback Method
tc	617.59	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	31.50	kJ/mol	265.50	NIST Webbook
hvapt	37.40	kJ/mol	350.50	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=C556616&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature