Propane, 2-isothiocyanato-2-methyl-

Other names:	tert-Butyl Isothiocyanate
	Isothiocyanic acid, tert-butyl ester
	t-Butyl isothiocyanate
Inchi:	InChI=1S/C5H9NS/c1-5(2,3)6-4-7/h1-3H3
InchiKey:	ZFWFRTVIIMTOLY-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CC(C)(C)N=C=S
Mol. weight [g/mol]:	115.20
CAS:	590-42-1

Physical Properties

Property code	Value	Unit	Source
hf	128.79	kJ/mol	Joback Method
hvap	35.87	kJ/mol	Joback Method
ie	9.06	eV	NIST Webbook
log10ws	-1.96		Crippen Method
logp	1.888		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	456.52	K	Joback Method
tc	689.64	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590421&Units=SI

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