Isobutyl isothiocyanate

Other names:	Propane, 1-isothiocyanato-2-methyl-
	Isothiocyanic acid, isobutyl ester
	i-Butyl isothiocyanate
	2-Methylpropyl isothiocyanate
Inchi:	InChI=1S/C5H9NS/c1-5(2)3-6-4-7/h5H,3H2,1-2H3
InchiKey:	NSDDRJXKROCWRZ-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CC(C)CN=C=S
Mol. weight [g/mol]:	115.20
CAS:	591-82-2

Physical Properties

Property code	Value	Unit	Source
hf	132.26	kJ/mol	Joback Method
hvap	36.78	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.745		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	921.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	926.00		NIST Webbook
tb	459.31	K	Joback Method
tc	682.31	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591822&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature