Butane, 1-isothiocyanato-

Other names:	Isothiocyanic acid, butyl ester
	Butyl isothiocyanate
	Butyl mustard oil
	n-Butyl isothiocyanate
	Isothiocyanic acid n-butyl ester
	1-Isothiocyanatobutane
Inchi:	InChI=1S/C5H9NS/c1-2-3-4-6-5-7/h2-4H2,1H3
InchiKey:	LIMQQADUEULBSO-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CCCCN=C=S
Mol. weight [g/mol]:	115.20
CAS:	592-82-5

Physical Properties

Property code	Value	Unit	Source
hf	137.54	kJ/mol	Joback Method
hvap	37.16	kJ/mol	Joback Method
ie	9.02 ± 0.05	eV	NIST Webbook
log10ws	-1.85		Crippen Method
logp	1.889		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	979.30		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	979.30		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	946.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1283.00		NIST Webbook
ripol	1308.00		NIST Webbook
tb	459.75	K	Joback Method
tc	677.45	K	Joback Method

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=C592825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature