Butane, 2-isothiocyanato-

Other names:	Isothiocyanic acid, sec-butyl ester
	sec-Butyl Isothiocyanate
	2-Butyl isothiocyanate
	1-Methylpropyl isothiocyanate
Inchi:	InChI=1S/C5H9NS/c1-3-5(2)6-4-7/h5H,3H2,1-2H3
InchiKey:	TUFJIDJGIQOYFY-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CCC(C)N=C=S
Mol. weight [g/mol]:	115.20
CAS:	4426-79-3

Physical Properties

Property code	Value	Unit	Source
hf	132.26	kJ/mol	Joback Method
hvap	36.78	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.888		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	937.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	933.30		NIST Webbook
rinpol	913.00		NIST Webbook
ripol	1287.00		NIST Webbook
tb	459.31	K	Joback Method
tc	682.31	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=C4426793&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature