Butane, 1-isothiocyanato-3-methyl-

Other names: 3-Methylbutyl isothiocyanate
Inchi: InChI=1S/C6H11NS/c1-6(2)3-4-7-5-8/h6H,3-4H2,1-2H3
InchiKey: JATNWMBUDXLMEO-UHFFFAOYSA-N
Formula: C6H11NS
SMILES: CC(C)CCN=C=S
Mol. weight [g/mol]: 129.22
CAS: 628-03-5

Physical Properties

Property code	Value	Unit	Source
hf	111.62	kJ/mol	Joback Method
hvap	39.00	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.135		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1040.70		NIST Webbook
ripol	1418.00		NIST Webbook
tb	482.19	K	Joback Method
tc	701.74	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628035&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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