Thiocyanic acid, butyl ester

Other names:	Butyl thiocyanate
	1-Thiocyanatobutane
	n-Butylthiocyanate
	n-Butyl rhodanate
	Butyrhodanid
	Butylthiokyanat
Inchi:	InChI=1S/C5H9NS/c1-2-3-4-7-5-6/h2-4H2,1H3
InchiKey:	HXNXAEYAXNPLHJ-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CCCCSC#N
Mol. weight [g/mol]:	115.20
CAS:	628-83-1

Physical Properties

Property code	Value	Unit	Source
gf	157.52	kJ/mol	Joback Method
hf	60.22	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	44.02	kJ/mol	Joback Method
ie	9.64 ± 0.05	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.001		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	484.66	K	Joback Method
tc	698.19	K	Joback Method
tf	245.50	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.75	J/mol×K	484.66	Joback Method
cpg	201.33	J/mol×K	520.25	Joback Method

cpg	209.52	J/mol×K	555.84	Joback Method
cpg	217.32	J/mol×K	591.43	Joback Method
cpg	224.73	J/mol×K	627.01	Joback Method
cpg	231.77	J/mol×K	662.60	Joback Method
cpg	238.43	J/mol×K	698.19	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628831&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

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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
tf: Normal melting (fusion) point
vc: Critical Volume