Thiocyanic acid, 2-propenyl ester

Other names:	Allylrhodanid
	Allyl thiocyanate
	Thiocyanic acid, allyl ester
Inchi:	InChI=1S/C4H5NS/c1-2-3-6-4-5/h2H,1,3H2
InchiKey:	IFVYHJRLWCUVBB-UHFFFAOYSA-N
Formula:	C4H5NS
SMILES:	C=CCSC#N
Mol. weight [g/mol]:	99.15
CAS:	764-49-8

Physical Properties

Property code	Value	Unit	Source
gf	236.94	kJ/mol	Joback Method
hf	206.29	kJ/mol	Joback Method
hfus	10.47	kJ/mol	Joback Method
hvap	41.12	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.387		Crippen Method
mcvol	80.650	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
ripol	1440.00		NIST Webbook
ripol	1440.00		NIST Webbook
tb	458.46	K	Joback Method
tc	680.21	K	Joback Method
tf	232.47	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.52	J/mol×K	458.46	Joback Method
cpg	144.72	J/mol×K	495.42	Joback Method
cpg	150.61	J/mol×K	532.38	Joback Method
cpg	156.18	J/mol×K	569.33	Joback Method

cpg	161.45	J/mol×K	606.29	Joback Method
cpg	166.42	J/mol×K	643.25	Joback Method
cpg	171.10	J/mol×K	680.21	Joback Method

Sources

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=C764498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume