

Trifluoromethylthiocyanate

Other names:	Thiocyanic acid, trifluoromethyl ester
Inchi:	InChI=1S/C2F3NS/c3-2(4,5)7-1-6
InchiKey:	IWJODGXJDSWIHQ-UHFFFAOYSA-N
Formula:	C2F3NS
SMILES:	N#CSC(F)(F)F
Mol. weight [g/mol]:	127.09
CAS:	690-24-4

Physical Properties

Property code	Value	Unit	Source
gf	-449.33	kJ/mol	Joback Method
hf	-474.94	kJ/mol	Joback Method
hfus	8.40	kJ/mol	Joback Method
hvap	33.59	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.720		Crippen Method
mcvol	62.080	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
tb	410.60	K	Joback Method
tc	611.33	K	Joback Method
tf	215.88	K	Joback Method
vc	0.271	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.24	J/mol×K	410.60	Joback Method
cpg	117.27	J/mol×K	444.06	Joback Method
cpg	120.97	J/mol×K	477.51	Joback Method
cpg	124.37	J/mol×K	510.97	Joback Method
cpg	127.47	J/mol×K	544.42	Joback Method
cpg	130.29	J/mol×K	577.88	Joback Method
cpg	132.85	J/mol×K	611.33	Joback Method
hvapt	32.60	kJ/mol	260.00	NIST Webbook

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=C690244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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