

Methane, tris(methylthio)-

Other names:	Orthoformic acid, trithio-, trimethyl ester Methyl orthotrithioformate Trimethyl trithioorthoformate Tris(methylthio)methane Trithiomethoxymethane Tris(methylthio)methane
Inchi:	InChI=1S/C4H10S3/c1-5-4(6-2)7-3/h4H,1-3H3
InchiKey:	YFMZQCCTZUJXEB-UHFFFAOYSA-N
Formula:	C4H10S3
SMILES:	CSC(SC)SC
Mol. weight [g/mol]:	154.32
CAS:	5418-86-0

Physical Properties

Property code	Value	Unit	Source
gf	79.72	kJ/mol	Joback Method
hf	-5.56	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.359		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1365.00		NIST Webbook
rinpol	1365.00		NIST Webbook
tb	496.82	K	Joback Method
tc	745.77	K	Joback Method
tf	223.04	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.04	J/mol×K	496.82	Joback Method

cpg	227.67	J/mol×K	538.31	Joback Method
cpg	237.77	J/mol×K	579.80	Joback Method
cpg	247.33	J/mol×K	621.29	Joback Method
cpg	256.33	J/mol×K	662.79	Joback Method
cpg	264.74	J/mol×K	704.28	Joback Method
cpg	272.55	J/mol×K	745.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.20	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5418860&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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