Carbonotrithioic acid, dimethyl ester

Other names:	Carbonic acid, trithio-, dimethyl ester
	Dimethyl trithiocarbonate
	(CH3S)2CS
	Dimethylester kyseliny trithiouhlicite
	Trithiocarbonic acid dimethyl ester
Inchi:	InChI=1S/C3H6S3/c1-5-3(4)6-2/h1-2H3
InchiKey:	IQWMXKTYXNMSLC-UHFFFAOYSA-N
Formula:	C3H6S3
SMILES:	CSC(=S)SC
Mol. weight [g/mol]:	138.28
CAS:	2314-48-9

Physical Properties

Property code	Value	Unit	Source
chl	-3836.00 ± 4.20	kJ/mol	NIST Webbook
gf	157.68	kJ/mol	Joback Method
hf	57.70	kJ/mol	NIST Webbook
hfl	-8.40 ± 4.20	kJ/mol	NIST Webbook
hfus	16.39	kJ/mol	Joback Method
hvap	66.27	kJ/mol	NIST Webbook
hvap	66.10	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	1.997		Crippen Method
mcvol	97.880	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
rinpol	1195.80		NIST Webbook
rinpol	1195.80		NIST Webbook
tb	475.64	K	Joback Method
tc	730.36	K	Joback Method
tf	266.90 ± 0.60	K	NIST Webbook
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.88	J/mol×K	475.64	Joback Method
cpg	169.20	J/mol×K	518.09	Joback Method
cpg	175.97	J/mol×K	560.55	Joback Method
cpg	182.23	J/mol×K	603.00	Joback Method
cpg	188.01	J/mol×K	645.45	Joback Method
cpg	193.34	J/mol×K	687.91	Joback Method
cpg	198.26	J/mol×K	730.36	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2314489&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume