Trithiomethane, methyl

Inchi: InChI=1S/C2H6S3/c1-5-2(3)4/h2-4H,1H3
InchiKey: WNYJLAZPCLYYRD-UHFFFAOYSA-N
Formula: C2H6S3
SMILES: CSC(S)S
Mol. weight [g/mol]: 126.26

Physical Properties

Property code	Value	Unit	Source
gf	55.42	kJ/mol	Joback Method
hf	28.94	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	39.95	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.493		Crippen Method
mcvol	88.090	ml/mol	McGowan Method
pc	6328.92	kPa	Joback Method
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
tb	439.22	K	Joback Method
tc	698.80	K	Joback Method
tf	204.62	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.74	J/mol×K	439.22	Joback Method
cpg	146.68	J/mol×K	482.48	Joback Method
cpg	153.25	J/mol×K	525.75	Joback Method
cpg	159.45	J/mol×K	569.01	Joback Method
cpg	165.27	J/mol×K	612.27	Joback Method
cpg	170.72	J/mol×K	655.53	Joback Method
cpg	175.78	J/mol×K	698.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62485&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
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