

Dimethyl trisulfide

Other names:	Trisulfide, dimethyl Methyl trisulfide CH3SSSCH3 2,3,4-Trithiapentane Dimethyl trisulphide dimethyl trisufide DMTS
Inchi:	InChI=1S/C2H6S3/c1-3-5-4-2/h1-2H3
InchiKey:	YWHLKYXPLRWGSE-UHFFFAOYSA-N
Formula:	C2H6S3
SMILES:	CSSSC
Mol. weight [g/mol]:	126.26
CAS:	3658-80-8

Physical Properties

Property code	Value	Unit	Source
gf	65.32	kJ/mol	Joback Method
hf	41.00	kJ/mol	Joback Method
hfus	13.33	kJ/mol	Joback Method
hvap	40.50	kJ/mol	Joback Method
ie	8.80 ± 0.15	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.73 ± 0.03	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.276		Crippen Method
mcvol	88.090	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
rinpol	948.00		NIST Webbook
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ripol	1357.00		NIST Webbook
tb	451.50	K	Joback Method
tc	703.73	K	Joback Method
tf	215.50	K	Joback Method
vc	0.309	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.59	J/mol×K	451.50	Joback Method
cpg	147.46	J/mol×K	493.54	Joback Method
cpg	154.10	J/mol×K	535.58	Joback Method
cpg	160.46	J/mol×K	577.62	Joback Method
cpg	166.52	J/mol×K	619.65	Joback Method
cpg	172.25	J/mol×K	661.69	Joback Method
cpg	177.60	J/mol×K	703.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3658808&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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