tert-Butyl Methyl disulfide

Other names:	Methyl tert-butyl disulphide
	Disulfide, tert-butyl methyl
	Methyl tert-butyl disulfide
	2-Methyl-2-propyl methyl disulfide
	Disulfide, 1,1-dimethylethyl methyl
	2,2-Dimethyl-3,4-dithiapentane
	Methyl t-butyl disulfide
Inchi:	InChI=1S/C5H12S2/c1-5(2,3)7-6-4/h1-4H3
InchiKey:	JEGYOGCWPYGLIB-UHFFFAOYSA-N
Formula:	C5H12S2
SMILES:	CSSC(C)(C)C
Mol. weight [g/mol]:	136.28
CAS:	35166-82-6

Physical Properties

Property code	Value	Unit	Source
gf	60.30	kJ/mol	Joback Method
hf	-112.00	kJ/mol	NIST Webbook
hfus	9.55	kJ/mol	Joback Method
hvap	39.06	kJ/mol	Joback Method
ie	8.40 ± 0.80	eV	NIST Webbook
log10ws	-2.79		Crippen Method
logp	2.796		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	950.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	950.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1238.00		NIST Webbook
tb	448.13	K	Joback Method
tc	678.67	K	Joback Method
tf	217.33	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.67	J/mol×K	448.13	Joback Method
cpg	228.91	J/mol×K	486.55	Joback Method
cpg	240.43	J/mol×K	524.98	Joback Method
cpg	251.25	J/mol×K	563.40	Joback Method
cpg	261.40	J/mol×K	601.82	Joback Method
cpg	270.88	J/mol×K	640.25	Joback Method
cpg	279.73	J/mol×K	678.67	Joback Method

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=C35166826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume