Disulfide, methyl 1-propenyl

Other names:	1-(Methyldisulfanyl)-1-propene
	1-propenyl methyl disulfide
	Methyl 1-propenyl disulfide
	Methyl-1-propenyl disulphide
	Methyl propenyl disulfide
	Disulfide, methyl propenyl
	Methyl 1-propenyl disulfide, (E)-
	methyl prop-1-enyl disulphide
Inchi:	InChI=1S/C4H8S2/c1-3-4-6-5-2/h3-4H,1-2H3
InchiKey:	FUDUFCLRGSEHAJ-UHFFFAOYSA-N
Formula:	C4H8S2
SMILES:	CC=CSSC
Mol. weight [g/mol]:	120.24
CAS:	5905-47-5

Physical Properties

Property code	Value	Unit	Source
gf	129.26	kJ/mol	Joback Method
hf	75.07	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	38.09	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.531		Crippen Method
mcvol	95.620	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
rinpol	910.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	902.00		NIST Webbook

rinpol	921.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1274.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1269.00		NIST Webbook
ripol	1269.00		NIST Webbook
ripol	1263.00		NIST Webbook
tb	432.64	K	Joback Method
tc	662.52	K	Joback Method
tf	198.56	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.54	J/mol×K	432.64	Joback Method
cpg	168.42	J/mol×K	470.95	Joback Method
cpg	176.85	J/mol×K	509.27	Joback Method
cpg	184.83	J/mol×K	547.58	Joback Method
cpg	192.36	J/mol×K	585.89	Joback Method
cpg	199.47	J/mol×K	624.20	Joback Method
cpg	206.15	J/mol×K	662.52	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5905475&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume