Disulfide, methyl 2-propenyl

Other names:	2-propenylmethyldisulfide
	4,5-dithia-1-hexene
	Allyl methyl disulfide
	Allyl methyl disulphide
	Methyl 2-propenyl disulfide
	Methyl allyl disulfide
	Methyl allyl disulphide
Inchi:	InChI=1S/C4H8S2/c1-3-4-6-5-2/h3H,1,4H2,2H3
InchiKey:	XNZOTQPMYMCTBZ-UHFFFAOYSA-N
Formula:	C4H8S2
SMILES:	C=CCSSC
Mol. weight [g/mol]:	120.24
CAS:	2179-58-0

Physical Properties

Property code	Value	Unit	Source
gf	136.88	kJ/mol	Joback Method
hf	83.28	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	37.46	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.184		Crippen Method
mcvol	95.620	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	895.00		NIST Webbook
rinpol	918.50		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	912.00		NIST Webbook

rinpol	920.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	918.50		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	900.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1283.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1241.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1271.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1271.00		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1241.00		NIST Webbook
ripol	1261.00		NIST Webbook
tb	425.16	K	Joback Method
tc	648.50	K	Joback Method
tf	201.88	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.63	J/mol×K	425.16	Joback Method
cpg	169.22	J/mol×K	462.38	Joback Method

cpg	177.43	J/mol×K	499.61	Joback Method
cpg	185.25	J/mol×K	536.83	Joback Method
cpg	192.69	J/mol×K	574.05	Joback Method
cpg	199.75	J/mol×K	611.28	Joback Method
cpg	206.42	J/mol×K	648.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2179580&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

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