Sulfide, allyl methyl

Other names:	1-Propene, 3-(methylthio)-
	Allyl methyl sulfide
	Methyl allyl sulfide
	3-(Methylthio)propene
	CH3SCH2CH=CH2
	3-(Methylsulfanyl)-1-propene
	3-(Methylthio)-1-propene
	Methyl 2-propenyl sulfide
	Methyl allyl sulphide
	allyl methyl sulphide
Inchi:	InChI=1S/C4H8S/c1-3-4-5-2/h3H,1,4H2,2H3
InchiKey:	NVLPQIPTCCLBEU-UHFFFAOYSA-N
Formula:	C4H8S
SMILES:	C=CCSC
Mol. weight [g/mol]:	88.17
CAS:	10152-76-8

Physical Properties

Property code	Value	Unit	Source
gf	103.76	kJ/mol	Joback Method
hf	41.41	kJ/mol	Joback Method
hfus	8.97	kJ/mol	Joback Method
hvap	30.65	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	8.70 ± 0.20	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
log10ws	-1.23		Crippen Method
logp	1.535		Crippen Method
mcvol	79.270	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	697.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	678.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	698.00		NIST Webbook

rinpol	696.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	698.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	976.00		NIST Webbook
ripol	948.00		NIST Webbook
ripol	943.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	932.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	960.00		NIST Webbook
ripol	956.00		NIST Webbook
tb	365.00	K	NIST Webbook
tb	365.20	K	NIST Webbook
tc	551.75	K	Joback Method
tf	167.48	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.29	J/mol×K	356.38	Joback Method
cpg	130.03	J/mol×K	388.94	Joback Method
cpg	137.45	J/mol×K	421.50	Joback Method
cpg	144.57	J/mol×K	454.07	Joback Method
cpg	151.40	J/mol×K	486.63	Joback Method
cpg	157.93	J/mol×K	519.19	Joback Method
cpg	164.17	J/mol×K	551.75	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=C10152768&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
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