Allyl mercaptan

Other names:	2-Propene-1-thiol
	Allylthiol
	CH2=CHCH2SH
	2-Propenyl-1-thiol
	2-Propenyl mercaptan
	prop-2-ene-1-thiol
Inchi:	InChI=1S/C3H6S/c1-2-3-4/h2,4H,1,3H2
InchiKey:	ULIKDJVNUXNQHS-UHFFFAOYSA-N
Formula:	C3H6S
SMILES:	C=CCS
Mol. weight [g/mol]:	74.14
CAS:	870-23-5

Physical Properties

Property code	Value	Unit	Source
gf	91.61	kJ/mol	Joback Method
hf	58.66	kJ/mol	Joback Method
hfus	6.29	kJ/mol	Joback Method
hvap	28.34	kJ/mol	Joback Method
ie	9.25	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
log10ws	-1.00		Crippen Method
logp	1.102		Crippen Method
mcvol	65.180	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
rinpol	579.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	575.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	593.00		NIST Webbook
rinpol	583.00		NIST Webbook
rinpol	580.00		NIST Webbook

rinpol	603.00		NIST Webbook
rinpol	603.00		NIST Webbook
ripol	891.00		NIST Webbook
ripol	904.00		NIST Webbook
ripol	895.00		NIST Webbook
ripol	901.00		NIST Webbook
ripol	904.00		NIST Webbook
ripol	895.00		NIST Webbook
ripol	901.00		NIST Webbook
ripol	863.00		NIST Webbook
ripol	887.00		NIST Webbook
tb	363.00 ± 6.00	K	NIST Webbook
tb	340.70	K	NIST Webbook
tb	342.00	K	NIST Webbook
tb	340.00 ± 3.00	K	NIST Webbook
tc	522.92	K	Joback Method
tf	158.27	K	Joback Method
vc	0.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.91	J/mol×K	327.58	Joback Method
cpg	96.96	J/mol×K	360.14	Joback Method
cpg	102.73	J/mol×K	392.69	Joback Method
cpg	108.23	J/mol×K	425.25	Joback Method
cpg	113.46	J/mol×K	457.80	Joback Method
cpg	118.45	J/mol×K	490.36	Joback Method
cpg	123.18	J/mol×K	522.92	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=C870235&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