

allyl hydrogen disulfide

Inchi:	InChI=1S/C3H6S2/c1-2-3-5-4/h2,4H,1,3H2
InchiKey:	VVYGQCSDUHWFGO-UHFFFAOYSA-N
Formula:	C3H6S2
SMILES:	C=CCSS
Mol. weight [g/mol]:	106.21

Physical Properties

Property code	Value	Unit	Source
gf	124.73	kJ/mol	Joback Method
hf	100.53	kJ/mol	Joback Method
hfus	10.42	kJ/mol	Joback Method
hvap	35.16	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.750		Crippen Method
mcvol	81.530	ml/mol	McGowan Method
pc	5228.24	kPa	Joback Method
rinpola	844.00		NIST Webbook
tb	396.36	K	Joback Method
tc	622.53	K	Joback Method
tf	192.67	K	Joback Method
vc	0.292	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.34	J/mol×K	396.36	Joback Method
cpg	132.15	J/mol×K	434.06	Joback Method
cpg	138.63	J/mol×K	471.75	Joback Method
cpg	144.78	J/mol×K	509.45	Joback Method
cpg	150.60	J/mol×K	547.14	Joback Method
cpg	156.11	J/mol×K	584.84	Joback Method
cpg	161.30	J/mol×K	622.53	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=R225864&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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