Allyl propyl sulfide

Other names:	4-thia-1-heptene
	2-propenyl propyl sulfide
	CH3CH2CH2SCH2CH=CH2
	3-(propylthio)propene
Inchi:	InChI=1S/C6H12S/c1-3-5-7-6-4-2/h3H,1,4-6H2,2H3
InchiKey:	JMLIYQJQKZYHDQ-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	C=CCSCCC
Mol. weight [g/mol]:	116.22
CAS:	27817-67-0

Physical Properties

Property code	Value	Unit	Source
gf	120.60	kJ/mol	Joback Method
hf	0.13	kJ/mol	Joback Method
hfus	14.15	kJ/mol	Joback Method
hvap	35.10	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.316		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	825.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	872.00		NIST Webbook
ripol	1099.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1099.00		NIST Webbook
ripol	1137.00		NIST Webbook
ripol	1099.00		NIST Webbook
tb	402.14	K	Joback Method
tc	595.12	K	Joback Method

tf	190.02	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.61	J/mol×K	402.14	Joback Method
cpg	202.42	J/mol×K	434.30	Joback Method
cpg	212.76	J/mol×K	466.47	Joback Method
cpg	222.66	J/mol×K	498.63	Joback Method
cpg	232.13	J/mol×K	530.79	Joback Method
cpg	241.16	J/mol×K	562.96	Joback Method
cpg	249.79	J/mol×K	595.12	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=C27817670&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
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