1-(1-Propenyl)-2-(4-thiohept-5-yl)disulfide

Other names: 1-(Propylthio)propyl 1-propenyl disulfide
Inchi: InChI=1S/C9H18S3/c1-4-7-10-9(6-3)12-11-8-5-2/h5,8-9H,4,6-7H2,1-3H3/b8-5+
InchiKey: ZJSMHYXMALNRQK-VMPITWQZSA-N
Formula: C9H18S3
SMILES: CC=CSSC(CC)SCCC
Mol. weight [g/mol]: 222.43

Physical Properties

Property code	Value	Unit	Source
gf	202.04	kJ/mol	Joback Method
hf	8.46	kJ/mol	Joback Method
hfus	28.13	kJ/mol	Joback Method
hvap	55.65	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.781		Crippen Method
mcvol	182.420	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	615.38	K	Joback Method
tc	850.66	K	Joback Method
tf	274.31	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.06	J/mol×K	615.38	Joback Method
cpg	437.42	J/mol×K	654.59	Joback Method
cpg	451.81	J/mol×K	693.81	Joback Method
cpg	465.26	J/mol×K	733.02	Joback Method
cpg	477.78	J/mol×K	772.23	Joback Method
cpg	489.40	J/mol×K	811.45	Joback Method
cpg	500.14	J/mol×K	850.66	Joback Method

Sources

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=U322309&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume