trans-Propenyl propyl disulfide

Inchi: InChI=1S/C6H12S2/c1-3-5-7-8-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey: AAPBYIVJOWCMGH-HWKANZROSA-N
Formula: C6H12S2
SMILES: CC=CSSCCC
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	146.10	kJ/mol	Joback Method
hf	33.79	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	42.54	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.311		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1118.00		NIST Webbook
tb	478.40	K	Joback Method
tc	701.27	K	Joback Method
tf	221.10	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.88	J/mol×K	478.40	Joback Method
cpg	248.67	J/mol×K	515.55	Joback Method
cpg	259.83	J/mol×K	552.69	Joback Method
cpg	270.40	J/mol×K	589.84	Joback Method
cpg	280.37	J/mol×K	626.98	Joback Method
cpg	289.77	J/mol×K	664.13	Joback Method
cpg	298.61	J/mol×K	701.27	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=R612347&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
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