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	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1419.00		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:	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=R209273&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume