2-Propenyl propyl disulfide

Inchi: InChI=1S/C6H12S2/c1-3-5-7-8-6-4-2/h3H,1,4-6H2,2H3
InchiKey: FCSSPCOFDUKHPV-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: C=CCSSCCC
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	153.72	kJ/mol	Joback Method
hf	42.00	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.964		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1097.00		NIST Webbook
tb	470.92	K	Joback Method
tc	687.95	K	Joback Method
tf	224.42	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.15	J/mol×K	470.92	Joback Method
cpg	248.69	J/mol×K	507.09	Joback Method
cpg	259.67	J/mol×K	543.26	Joback Method
cpg	270.11	J/mol×K	579.43	Joback Method
cpg	280.01	J/mol×K	615.61	Joback Method
cpg	289.38	J/mol×K	651.78	Joback Method
cpg	298.22	J/mol×K	687.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R612218&Units=SI
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

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