2-Propen-1-ol, 3-(2-propenylthio)

Inchi: InChI=1S/C6H10OS/c1-2-5-8-6-3-4-7/h2-3,6-7H,1,4-5H2/b6-3+
InchiKey: LWYSEPBDBMVXNJ-ZZXKWVIFSA-N
Formula: C6H10OS
SMILES: C=CCSC=CCO
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
gf	64.00	kJ/mol	Joback Method
hf	-34.88	kJ/mol	Joback Method
hfus	18.44	kJ/mol	Joback Method
hvap	51.73	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.412		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	1038.00		NIST Webbook
tb	498.48	K	Joback Method
tc	690.88	K	Joback Method
tf	245.76	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.34	J/mol×K	498.48	Joback Method
cpg	228.20	J/mol×K	530.55	Joback Method
cpg	236.59	J/mol×K	562.61	Joback Method
cpg	244.53	J/mol×K	594.68	Joback Method
cpg	252.04	J/mol×K	626.75	Joback Method
cpg	259.14	J/mol×K	658.82	Joback Method
cpg	265.86	J/mol×K	690.88	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=R82384&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume