(E)-Allyl(prop-1-en-1-yl)sulfane

Inchi: InChI=1S/C6H10S/c1-3-5-7-6-4-2/h3-4,6H,1,5H2,2H3/b6-4+
InchiKey: GHMLMYZSPZIABJ-GQCTYLIASA-N
Formula: C6H10S
SMILES: C=CCSC=CC
Mol. weight [g/mol]: 114.21
CAS: 104324-36-9

Physical Properties

Property code	Value	Unit	Source
gf	200.82	kJ/mol	Joback Method
hf	117.35	kJ/mol	Joback Method
hfus	14.35	kJ/mol	Joback Method
hvap	35.06	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.439		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	890.90		NIST Webbook
rinpol	890.90		NIST Webbook
tb	406.30	K	Joback Method
tc	609.54	K	Joback Method
tf	184.94	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.33	J/mol×K	406.30	Joback Method
cpg	186.76	J/mol×K	440.17	Joback Method
cpg	196.65	J/mol×K	474.05	Joback Method
cpg	206.01	J/mol×K	507.92	Joback Method
cpg	214.86	J/mol×K	541.79	Joback Method
cpg	223.22	J/mol×K	575.66	Joback Method
cpg	231.13	J/mol×K	609.54	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=C104324369&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