(Z)-1-Allyl-3-(prop-1-en-1-yl)trisulfane

Inchi: InChI=1S/C6H10S3/c1-3-5-7-9-8-6-4-2/h3-4,6H,1,5H2,2H3/b6-4-
InchiKey: ABXMBMQLMGNKES-XQRVVYSFSA-N
Formula: C6H10S3
SMILES: C=CCSSSC=CC
Mol. weight [g/mol]: 178.34
CAS: 382161-75-3

Physical Properties

Property code	Value	Unit	Source
gf	267.06	kJ/mol	Joback Method
hf	201.09	kJ/mol	Joback Method
hfus	22.61	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.736		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
rinpol	1328.80		NIST Webbook
rinpol	1328.80		NIST Webbook
tb	543.86	K	Joback Method
tc	794.59	K	Joback Method
tf	253.74	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.38	J/mol×K	543.86	Joback Method
cpg	274.72	J/mol×K	585.65	Joback Method
cpg	285.31	J/mol×K	627.44	Joback Method
cpg	295.16	J/mol×K	669.22	Joback Method
cpg	304.31	J/mol×K	711.01	Joback Method
cpg	312.76	J/mol×K	752.80	Joback Method
cpg	320.53	J/mol×K	794.59	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=C382161753&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