allyl propyl tetrasulfide

Other names: Propyl 2-propenyl tetrasulfide
Inchi: InChI=1S/C6H12S4/c1-3-5-7-9-10-8-6-4-2/h3H,1,4-6H2,2H3
InchiKey: WMYACRLMJNCCQB-UHFFFAOYSA-N
Formula: C6H12S4
SMILES: C=CCSSSSCCC
Mol. weight [g/mol]: 212.42

Physical Properties

Property code	Value	Unit	Source
gf	219.96	kJ/mol	Joback Method
hf	125.74	kJ/mol	Joback Method
hfus	26.54	kJ/mol	Joback Method
hvap	55.55	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.260		Crippen Method
mcvol	156.500	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1520.00		NIST Webbook
tb	608.48	K	Joback Method
tc	867.68	K	Joback Method
tf	293.22	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.81	J/mol×K	608.48	Joback Method
cpg	340.11	J/mol×K	651.68	Joback Method
cpg	351.56	J/mol×K	694.88	Joback Method
cpg	362.13	J/mol×K	738.08	Joback Method
cpg	371.82	J/mol×K	781.28	Joback Method

cpg	380.61	J/mol×K	824.48	Joback Method
cpg	388.49	J/mol×K	867.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R53490&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