Propyl (E)-1-propenyl tetrasulfide

Other names: Propyl 1-propenyl tetrasulfide, (E)-
E-1-propenyl propyl tetrasulfide
Propyl (E)-propenyl tetrasulfide
propyl trans-propenyl tetrasulfide
Inchi: InChI=1S/C6H12S4/c1-3-5-7-9-10-8-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey: RKTJCWCBNXCDDQ-HWKANZROSA-N
Formula: C6H12S4
SMILES: CC=CSSSSCCC
Mol. weight [g/mol]: 212.42

Physical Properties

Property code	Value	Unit	Source
gf	212.34	kJ/mol	Joback Method
hf	117.53	kJ/mol	Joback Method
hfus	28.02	kJ/mol	Joback Method
hvap	56.18	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.608		Crippen Method
mcvol	156.500	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	615.96	K	Joback Method
tc	881.09	K	Joback Method
tf	289.90	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.36	J/mol×K	615.96	Joback Method
cpg	339.74	J/mol×K	660.15	Joback Method

cpg	351.21	J/mol×K	704.34	Joback Method
cpg	361.78	J/mol×K	748.52	Joback Method
cpg	371.45	J/mol×K	792.71	Joback Method
cpg	380.21	J/mol×K	836.90	Joback Method
cpg	388.05	J/mol×K	881.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R53468&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