trans-Propenyl propyl trisulfide

Inchi: InChI=1S/C6H12S3/c1-3-5-7-9-8-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey: CKVNYTRYOFXVGM-HWKANZROSA-N
Formula: C6H12S3
SMILES: CC=CSSSCCC
Mol. weight [g/mol]: 180.35

Physical Properties

Property code	Value	Unit	Source
gf	179.22	kJ/mol	Joback Method
hf	75.66	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.960		Crippen Method
mcvol	140.150	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1333.00		NIST Webbook
rinpol	1333.00		NIST Webbook
tb	547.18	K	Joback Method
tc	792.12	K	Joback Method
tf	255.50	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.26	J/mol×K	547.18	Joback Method
cpg	294.48	J/mol×K	588.00	Joback Method
cpg	305.95	J/mol×K	628.83	Joback Method
cpg	316.70	J/mol×K	669.65	Joback Method
cpg	326.73	J/mol×K	710.47	Joback Method
cpg	336.04	J/mol×K	751.29	Joback Method
cpg	344.66	J/mol×K	792.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R637099&Units=SI

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