1,2,4-Trithiolane, 3,5-bis-(1-methylethyl), #1

Inchi: InChI=1S/C8H16S3/c1-5(2)7-9-8(6(3)4)11-10-7/h5-8H,1-4H3
InchiKey: QCTAPVCDZUSECS-UHFFFAOYSA-N
Formula: C8H16S3
SMILES: CC(C)C1SSC(C(C)C)S1
Mol. weight [g/mol]: 208.41

Physical Properties

Property code	Value	Unit	Source
gf	160.02	kJ/mol	Joback Method
hf	-43.09	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.079		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1444.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1775.00		NIST Webbook
tb	535.66	K	Joback Method
tc	782.11	K	Joback Method
tf	406.93	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.09	J/mol×K	535.66	Joback Method
cpg	377.71	J/mol×K	576.73	Joback Method
cpg	394.19	J/mol×K	617.81	Joback Method
cpg	409.59	J/mol×K	658.88	Joback Method
cpg	423.94	J/mol×K	699.96	Joback Method

cpg	437.31	J/mol×K	741.03	Joback Method
cpg	449.74	J/mol×K	782.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62154&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume