3-ethyl-6-methyl-1,2,4-trithiane

Inchi: InChI=1S/C6H12S3/c1-3-6-7-4-5(2)8-9-6/h5-6H,3-4H2,1-2H3
InchiKey: ICYNGJARSYXIPB-UHFFFAOYSA-N
Formula: C6H12S3
SMILES: CCC1SCC(C)SS1
Mol. weight [g/mol]: 180.35

Physical Properties

Property code	Value	Unit	Source
gf	135.96	kJ/mol	Joback Method
hf	2.59	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	46.51	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.239		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
ripol	1848.00		NIST Webbook
tb	495.05	K	Joback Method
tc	749.46	K	Joback Method
tf	410.87	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.11	J/mol×K	495.05	Joback Method
cpg	285.81	J/mol×K	537.45	Joback Method
cpg	300.52	J/mol×K	579.85	Joback Method
cpg	314.28	J/mol×K	622.25	Joback Method
cpg	327.11	J/mol×K	664.66	Joback Method
cpg	339.04	J/mol×K	707.06	Joback Method
cpg	350.12	J/mol×K	749.46	Joback Method

Sources

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=R225775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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