2,4,6-Triethyl-1,3,5-trithiane

Inchi: InChI=1S/C9H18S3/c1-4-7-10-8(5-2)12-9(6-3)11-7/h7-9H,4-6H2,1-3H3
InchiKey: PHQSYHLEPPMJSU-UHFFFAOYSA-N
Formula: C9H18S3
SMILES: CCC1SC(CC)SC(CC)S1
Mol. weight [g/mol]: 222.43

Physical Properties

Property code	Value	Unit	Source
gf	153.51	kJ/mol	Joback Method
hf	-79.67	kJ/mol	Joback Method
hfus	24.01	kJ/mol	Joback Method
hvap	52.88	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.408		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpol	1560.70		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2040.00		NIST Webbook
tb	559.02	K	Joback Method
tc	798.16	K	Joback Method
tf	440.44	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.76	J/mol×K	559.02	Joback Method
cpg	427.79	J/mol×K	598.88	Joback Method
cpg	445.68	J/mol×K	638.73	Joback Method
cpg	462.47	J/mol×K	678.59	Joback Method
cpg	478.18	J/mol×K	718.44	Joback Method
cpg	492.85	J/mol×K	758.30	Joback Method
cpg	506.50	J/mol×K	798.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R494510&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume