4-methyl-1,2,5-trithiepane

Inchi: InChI=1S/C5H10S3/c1-5-4-8-7-3-2-6-5/h5H,2-4H2,1H3
InchiKey: RVOHMSHTYMGLHL-UHFFFAOYSA-N
Formula: C5H10S3
SMILES: CC1CSSCCS1
Mol. weight [g/mol]: 166.33

Physical Properties

Property code	Value	Unit	Source
gf	123.15	kJ/mol	Joback Method
hf	37.41	kJ/mol	Joback Method
hfus	9.41	kJ/mol	Joback Method
hvap	44.76	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.503		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	481.11	K	Joback Method
tc	751.75	K	Joback Method
tf	400.32	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.98	J/mol×K	481.11	Joback Method
cpg	241.07	J/mol×K	526.22	Joback Method
cpg	255.14	J/mol×K	571.32	Joback Method
cpg	268.20	J/mol×K	616.43	Joback Method
cpg	280.29	J/mol×K	661.54	Joback Method
cpg	291.45	J/mol×K	706.64	Joback Method

cpg	301.69	J/mol×K	751.75	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=R222474&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