1,2,4,6-Tetrathiepane

Inchi: InChI=1S/C3H6S4/c1-4-2-6-7-3-5-1/h1-3H2
InchiKey: LCABDMYFXTZXMI-UHFFFAOYSA-N
Formula: C3H6S4
SMILES: C1SCSSCS1
Mol. weight [g/mol]: 170.34
CAS: 292-45-5

Physical Properties

Property code	Value	Unit	Source
gf	153.88	kJ/mol	Joback Method
hf	144.29	kJ/mol	Joback Method
hfus	6.82	kJ/mol	Joback Method
hvap	46.43	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.720		Crippen Method
mcvol	107.670	ml/mol	McGowan Method
pc	6229.41	kPa	Joback Method
rinpol	1489.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1489.00		NIST Webbook
ripol	2420.00		NIST Webbook
ripol	2420.00		NIST Webbook
tb	487.85	K	Joback Method
tc	788.29	K	Joback Method
tf	465.47	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.05	J/mol×K	487.85	Joback Method
cpg	194.41	J/mol×K	537.92	Joback Method
cpg	204.79	J/mol×K	588.00	Joback Method

cpg	214.24	J/mol×K	638.07	Joback Method
cpg	222.81	J/mol×K	688.14	Joback Method
cpg	230.56	J/mol×K	738.22	Joback Method
cpg	237.53	J/mol×K	788.29	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=C292455&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume