methyl-1,2,3,4-tetrathiane

Inchi: InChI=1S/C3H6S4/c1-3-2-4-6-7-5-3/h3H,2H2,1H3
InchiKey: MUHSSCIXCFPQHS-UHFFFAOYSA-N
Formula: C3H6S4
SMILES: CC1CSSSS1
Mol. weight [g/mol]: 170.34
CAS: 116664-30-3

Physical Properties

Property code	Value	Unit	Source
gf	158.27	kJ/mol	Joback Method
hf	130.11	kJ/mol	Joback Method
hfus	9.99	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.066		Crippen Method
mcvol	107.670	ml/mol	McGowan Method
pc	5695.98	kPa	Joback Method
rinpol	1335.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1369.30		NIST Webbook
rinpol	1369.30		NIST Webbook
rinpol	1359.00		NIST Webbook
ripol	2005.00		NIST Webbook
ripol	2005.00		NIST Webbook
tb	478.91	K	Joback Method
tc	766.95	K	Joback Method
tf	464.75	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.14	J/mol×K	478.91	Joback Method
cpg	196.91	J/mol×K	526.92	Joback Method

cpg	206.82	J/mol×K	574.92	Joback Method
cpg	215.92	J/mol×K	622.93	Joback Method
cpg	224.26	J/mol×K	670.94	Joback Method
cpg	231.88	J/mol×K	718.94	Joback Method
cpg	238.82	J/mol×K	766.95	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=C116664303&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