

Methyl 1,2,4,5-tetrathiane

Inchi:	InChI=1S/C3H6S4/c1-3-6-4-2-5-7-3/h3H,2H2,1H3
InchiKey:	VWHXUHVCDTGT-UHFFFAOYSA-N
Formula:	C3H6S4
SMILES:	CC1SSCSS1
Mol. weight [g/mol]:	170.34

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
mvol	107.670	ml/mol	McGowan Method
pc	5695.98	kPa	Joback Method
rinpol	1362.00		NIST Webbook
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tb	478.91	K	Joback Method
tc	766.95	K	Joback Method
tf	464.75	K	Joback Method
vc	0.321	m ³ /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/ci9903071
Crippen Method:	https://www.cheméo.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=R587256&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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