

1,2,4-Trithiolane, 3,3,5,5-tetramethyl-

Other names:	3,3,5,5-Tetramethyl-1,2,4-trithiolane 1,2,4-Trithiolane, tetramethyl-
Inchi:	InChI=1S/C6H12S3/c1-5(2)7-6(3,4)9-8-5/h1-4H3
InchiKey:	XFOWPRWOLKTTSD-UHFFFAOYSA-N
Formula:	C6H12S3
SMILES:	CC1(C)SSC(C)(C)S1
Mol. weight [g/mol]:	180.35
CAS:	38348-31-1

Physical Properties

Property code	Value	Unit	Source
gf	137.08	kJ/mol	Joback Method
hf	39.23	kJ/mol	Joback Method
hfus	4.68	kJ/mol	Joback Method
hvap	44.03	kJ/mol	Joback Method
ie	8.10 ± 0.20	eV	NIST Webbook
ie	8.12	eV	NIST Webbook
log10ws	-4.08		Crippen Method
logp	3.587		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1651.00		NIST Webbook
tb	491.26	K	Joback Method
tc	759.22	K	Joback Method
tf	462.19	K	Joback Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.26	J/mol×K	491.26	Joback Method

cpg	285.51	J/mol×K	535.92	Joback Method
cpg	298.24	J/mol×K	580.58	Joback Method
cpg	309.82	J/mol×K	625.24	Joback Method
cpg	320.63	J/mol×K	669.90	Joback Method
cpg	331.03	J/mol×K	714.56	Joback Method
cpg	341.40	J/mol×K	759.22	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=C38348311&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
ie:	Ionization energy
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

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