1,3,5-Trithiane, 2,2,4,4,6,6-hexamethyl-

Other names:	s-Trithiane, 2,2,4,4,6,6-hexamethyl-
	Hexamethyl-s-trithiane
	Trithioacetone
	2,2,4,4,6,6-Hexamethyl-s-trithiane
	Hexamethyl-1,3,5-trithiane
	2,2,4,4,6,6-Hexamethyl-s-trithiane (trithioacetone)
	2,2,4,4,6,6-hexamethyl-1,3,5-trithiane
Inchi:	InChI=1S/C9H18S3/c1-7(2)10-8(3,4)12-9(5,6)11-7/h1-6H3
InchiKey:	NBNWHQAWKFYFKI-UHFFFAOYSA-N
Formula:	C9H18S3
SMILES:	CC1(C)SC(C)(C)SC(C)(C)S1
Mol. weight [g/mol]:	222.43
CAS:	828-26-2

Physical Properties

Property code	Value	Unit	Source
gf	137.04	kJ/mol	Joback Method
hf	-33.95	kJ/mol	Joback Method
hfus	5.12	kJ/mol	Joback Method
hvap	49.42	kJ/mol	Joback Method
ie	7.95 ± 0.05	eV	NIST Webbook
log10ws	-4.96		Crippen Method
logp	4.408		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	559.74	K	Joback Method
tc	832.07	K	Joback Method
tf	512.14	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.52	J/mol×K	559.74	Joback Method

cpg	423.66	J/mol×K	605.13	Joback Method
cpg	440.44	J/mol×K	650.52	Joback Method
cpg	456.40	J/mol×K	695.90	Joback Method
cpg	472.10	J/mol×K	741.29	Joback Method
cpg	488.06	J/mol×K	786.68	Joback Method
cpg	504.84	J/mol×K	832.07	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=C828262&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume