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

Other names:	2,5-Dimethyl-1,3,4-trithiolane
	3,5-Dimethyl-1,2,4-trithiolane
	3,5-Dimethyl-1,2,4-trithiolan
	3,5-Methylethyl-1,2,4-trithiolane
	3,5-dimethyl-1,2,-trithiolane, isomer 1
	3,5-dimethyl-1,2,-trithiolane, isomer 2
Inchi:	InChI=1S/C4H8S3/c1-3-5-4(2)7-6-3/h3-4H,1-2H3
InchiKey:	HFRUNLRFNNTTPQ-UHFFFAOYSA-N
Formula:	C4H8S3
SMILES:	CC1SSC(C)S1
Mol. weight [g/mol]:	152.30
CAS:	23654-92-4

Physical Properties

Property code	Value	Unit	Source
gf	131.22	kJ/mol	Joback Method
hf	50.03	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	41.88	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.807		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1136.00		NIST Webbook

rinpol	1101.00		NIST Webbook
rinpol	1189.10		NIST Webbook
rinpol	1172.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1100.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1602.00		NIST Webbook
tb	445.02	K	Joback Method
tc	698.77	K	Joback Method
tf	391.85	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.82	J/mol×K	445.02	Joback Method
cpg	201.68	J/mol×K	487.31	Joback Method
cpg	212.78	J/mol×K	529.60	Joback Method
cpg	223.15	J/mol×K	571.90	Joback Method
cpg	232.82	J/mol×K	614.19	Joback Method
cpg	241.83	J/mol×K	656.48	Joback Method
cpg	250.21	J/mol×K	698.77	Joback Method

Sources

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=C23654924&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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